



# wwPDB X-ray Structure Validation Summary Report

Oct 23, 2021 – 08:37 AM EDT

PDB ID : 1FNT  
Title : CRYSTAL STRUCTURE OF THE 20S PROTEASOME FROM YEAST IN COMPLEX WITH THE PROTEASOME ACTIVATOR PA26 FROM TRY-PANOSOME BRUCEI AT 3.2 ANGSTROMS RESOLUTION  
Authors : Whitby, F.G.; Masters, E.; Kramer, L.; Knowlton, J.R.; Yao, Y.; Wang, C.C.; Hill, C.P.  
Deposited on : 2000-08-23  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

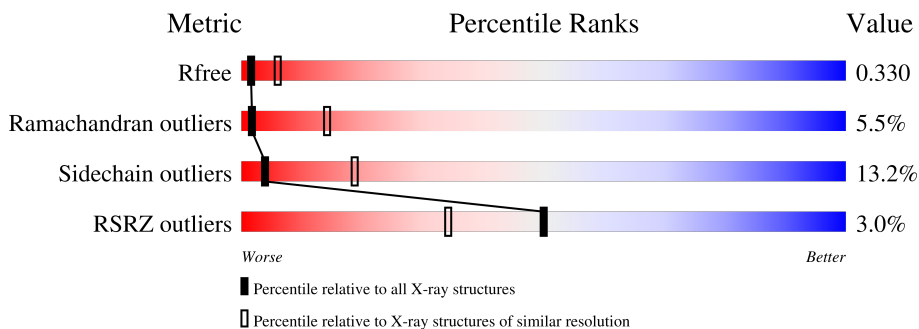
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



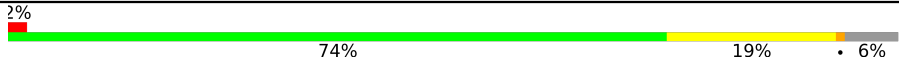
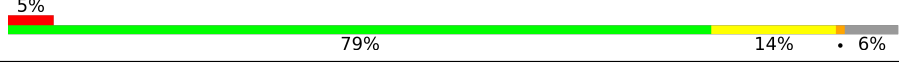
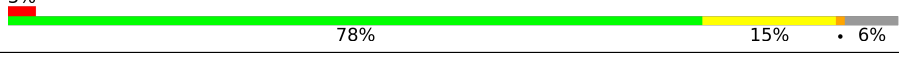


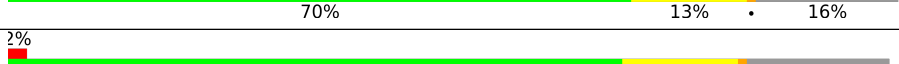
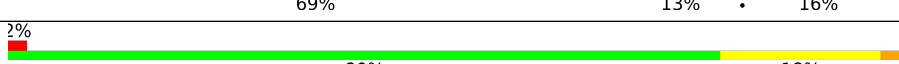
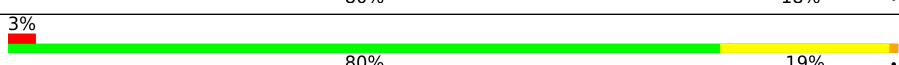
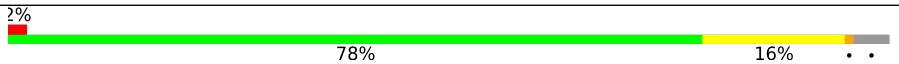


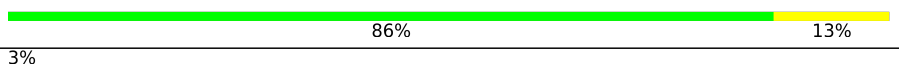
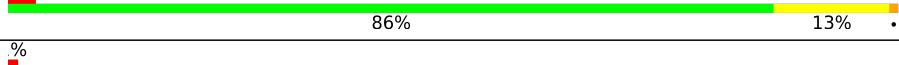

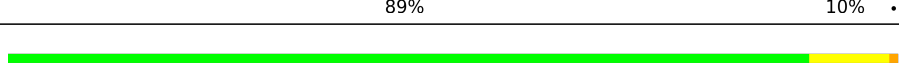
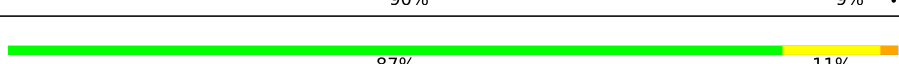









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	A	252	 3% 75% 18% • 6%
1	O	252	 2% 75% 18% • 6%
2	B	250	 2% 80% 18% ••
2	P	250	 % 79% 19% •
3	C	245	 2% 79% 17% ••
3	Q	245	 4% 80% 16% ••
4	D	254	 2% 74% 19% • 6%

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Mol	Chain	Length	Quality of chain
4	R	254	 2% 74% 19% 6%
5	E	260	 5% 79% 14% 6%
5	S	260	 3% 78% 15% 6%
6	F	234	 0% 85% 14% 0%
6	T	234	 0% 84% 15% 0%
7	G	287	 2% 70% 13% 16%
7	U	287	 2% 69% 13% 16%
8	H	196	 2% 80% 18% 0%
8	V	196	 3% 80% 19% 0%
9	I	232	 2% 78% 16% 0%
9	W	232	 2% 80% 16% 0%
10	J	205	 0% 86% 14% 0%
10	X	205	 0% 86% 13% 0%
11	K	198	 3% 86% 13% 0%
11	Y	198	 0% 85% 14% 0%
12	L	212	 0% 89% 10% 0%
12	Z	212	 0% 90% 9% 0%
13	M	222	 0% 87% 11% 0%
13	a	222	 0% 86% 12% 0%
14	N	233	 0% 80% 18% 0%
14	b	233	 0% 78% 20% 0%
15	c	231	 2% 74% 12% 14%
15	d	231	 8% 74% 12% 14%
15	e	231	 8% 74% 12% 14%
15	f	231	 3% 74% 12% 14%

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Mol	Chain	Length	Quality of chain
15	g	231	<p>3% 74% 12% 14%</p>
15	h	231	<p>3% 74% 12% 14%</p>
15	i	231	<p>3% 74% 12% 14%</p>
15	j	231	<p>4% 74% 12% 14%</p>
15	k	231	<p>5% 74% 12% 14%</p>
15	l	231	<p>6% 74% 12% 14%</p>
15	m	231	<p>6% 74% 12% 14%</p>
15	n	231	<p>4% 74% 12% 14%</p>
15	o	231	<p>5% 74% 12% 14%</p>
15	p	231	<p>9% 74% 11% 14%</p>

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 70622 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEASOME COMPONENT C7-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	238	Total	C	N	O	S	0	0	0
			1881	1197	314	362	8			
1	O	238	Total	C	N	O	S	0	0	0
			1881	1197	314	362	8			

- Molecule 2 is a protein called PROTEASOME COMPONENT Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	247	Total	C	N	O	S	0	0	0
			1868	1188	309	368	3			
2	P	247	Total	C	N	O	S	0	0	0
			1868	1188	309	368	3			

- Molecule 3 is a protein called PROTEASOME COMPONENT Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	Total	C	N	O	S	0	0	0
			1868	1180	312	373	3			
3	Q	241	Total	C	N	O	S	0	0	0
			1868	1180	312	373	3			

- Molecule 4 is a protein called PROTEASOME COMPONENT PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	239	Total	C	N	O	S	0	0	0
			1862	1163	326	369	4			
4	R	239	Total	C	N	O	S	0	0	0
			1862	1163	326	369	4			

- Molecule 5 is a protein called PROTEASOME COMPONENT PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1871	1168	316	380	7			
5	S	244	Total	C	N	O	S	0	0	0
			1871	1168	316	380	7			

- Molecule 6 is a protein called PROTEASOME COMPONENT PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
6	T	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 7 is a protein called PROTEASOME COMPONENT C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	240	Total	C	N	O	S	0	0	0
			1869	1188	326	351	4			
7	U	240	Total	C	N	O	S	0	0	0
			1869	1188	326	351	4			

- Molecule 8 is a protein called PROTEASOME COMPONENT PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			
8	V	196	Total	C	N	O	S	0	0	0
			1510	954	250	299	7			

- Molecule 9 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
9	W	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 10 is a protein called PROTEASOME COMPONENT PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	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	X	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	K	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			
11	Y	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	L	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			
12	Z	212	Total	C	N	O	S	0	0	0
			1646	1045	282	312	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	33	ARG	LYS	engineered mutation	UNP P30656
Z	33	ARG	LYS	engineered mutation	UNP P30656

- Molecule 13 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
13	a	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	N	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
14	b	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 15 is a protein called PROTEASOME ACTIVATOR PROTEIN PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	c	198	1529	960	267	296	6	0	0	0
15	d	198	1529	960	267	296	6	0	0	0
15	e	198	1529	960	267	296	6	0	0	0
15	f	198	1529	960	267	296	6	0	0	0
15	g	198	1529	960	267	296	6	0	0	0
15	h	198	1529	960	267	296	6	0	0	0
15	i	198	1529	960	267	296	6	0	0	0
15	j	198	1529	960	267	296	6	0	0	0
15	k	198	1529	960	267	296	6	0	0	0
15	l	198	1529	960	267	296	6	0	0	0
15	m	198	1529	960	267	296	6	0	0	0
15	n	198	1529	960	267	296	6	0	0	0
15	o	198	1529	960	267	296	6	0	0	0
15	p	198	1529	960	267	296	6	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	49	VAL	THR	see remark 999	UNP Q9U8G2
c	226	THR	SER	see remark 999	UNP Q9U8G2
d	49	VAL	THR	see remark 999	UNP Q9U8G2
d	226	THR	SER	see remark 999	UNP Q9U8G2
e	49	VAL	THR	see remark 999	UNP Q9U8G2
e	226	THR	SER	see remark 999	UNP Q9U8G2
f	49	VAL	THR	see remark 999	UNP Q9U8G2
f	226	THR	SER	see remark 999	UNP Q9U8G2
g	49	VAL	THR	see remark 999	UNP Q9U8G2
g	226	THR	SER	see remark 999	UNP Q9U8G2
h	49	VAL	THR	see remark 999	UNP Q9U8G2
h	226	THR	SER	see remark 999	UNP Q9U8G2

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Chain	Residue	Modelled	Actual	Comment	Reference
i	49	VAL	THR	see remark 999	UNP Q9U8G2
i	226	THR	SER	see remark 999	UNP Q9U8G2
j	49	VAL	THR	see remark 999	UNP Q9U8G2
j	226	THR	SER	see remark 999	UNP Q9U8G2
k	49	VAL	THR	see remark 999	UNP Q9U8G2
k	226	THR	SER	see remark 999	UNP Q9U8G2
l	49	VAL	THR	see remark 999	UNP Q9U8G2
l	226	THR	SER	see remark 999	UNP Q9U8G2
m	49	VAL	THR	see remark 999	UNP Q9U8G2
m	226	THR	SER	see remark 999	UNP Q9U8G2
n	49	VAL	THR	see remark 999	UNP Q9U8G2
n	226	THR	SER	see remark 999	UNP Q9U8G2
o	49	VAL	THR	see remark 999	UNP Q9U8G2
o	226	THR	SER	see remark 999	UNP Q9U8G2
p	49	VAL	THR	see remark 999	UNP Q9U8G2
p	226	THR	SER	see remark 999	UNP Q9U8G2

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	H	1	Total Mg 1 1	0	0
16	I	1	Total Mg 1 1	0	0
16	J	2	Total Mg 2 2	0	0
16	L	1	Total Mg 1 1	0	0
16	M	1	Total Mg 1 1	0	0
16	U	1	Total Mg 1 1	0	0
16	V	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0
16	X	2	Total Mg 2 2	0	0
16	Z	1	Total Mg 1 1	0	0

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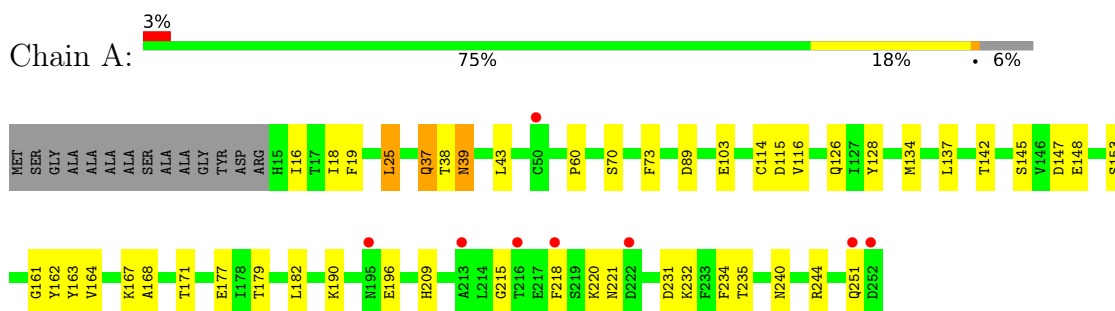
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
16	a	1	Total	Mg	0	0
			1	1		

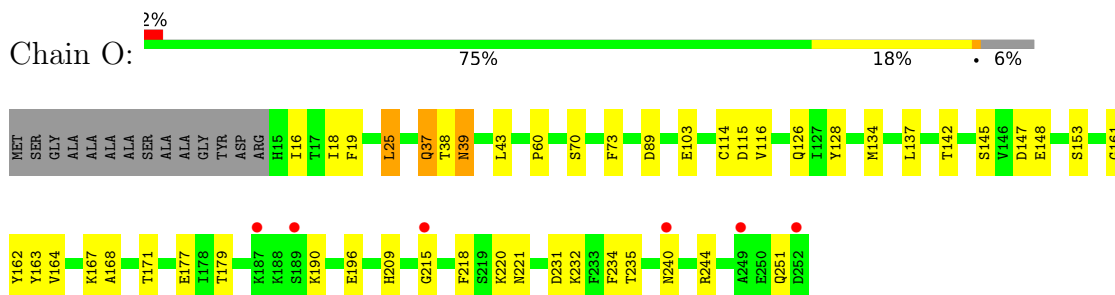
### 3 Residue-property plots i

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

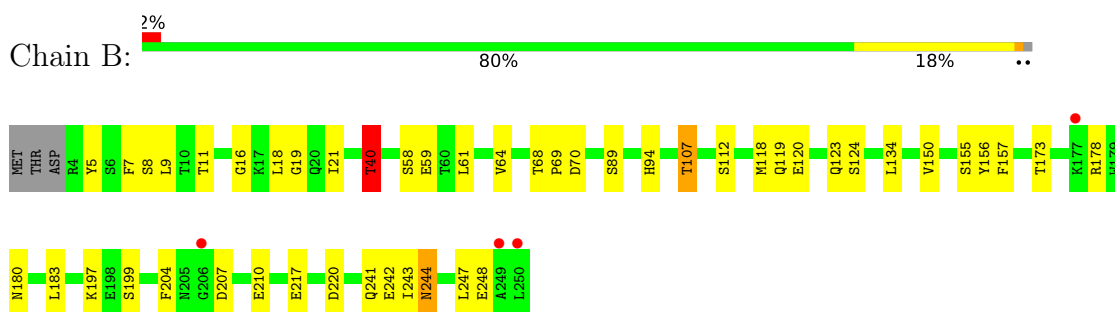
- Molecule 1: PROTEASOME COMPONENT C7-ALPHA



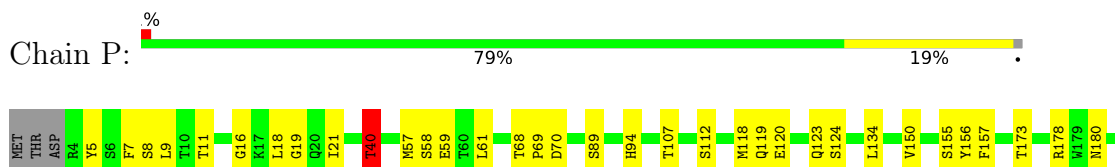
- Molecule 1: PROTEASOME COMPONENT C7-ALPHA



- Molecule 2: PROTEASOME COMPONENT Y7

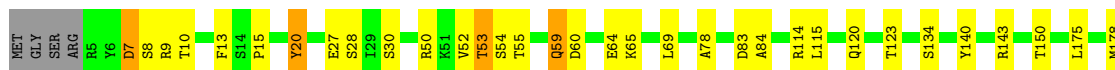
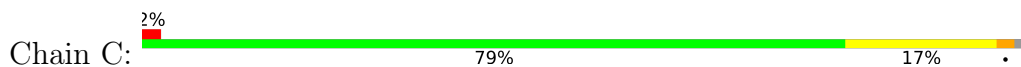


- Molecule 2: PROTEASOME COMPONENT Y7

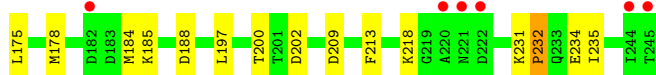
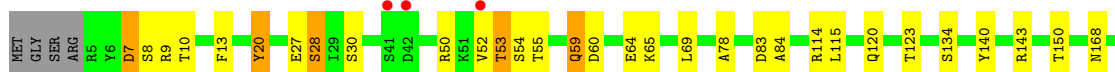
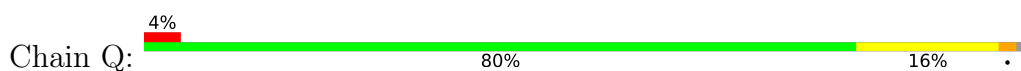




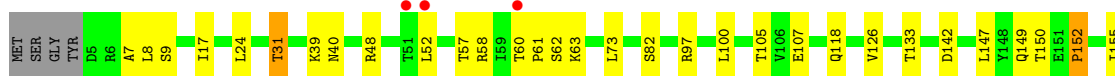
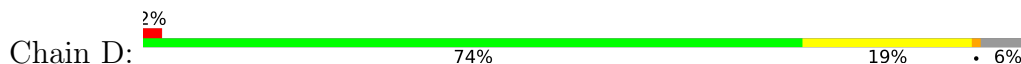
- Molecule 3: PROTEASOME COMPONENT Y13



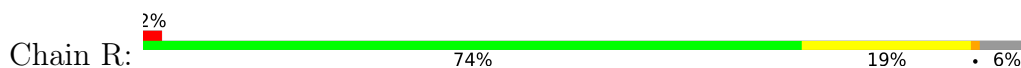
- Molecule 3: PROTEASOME COMPONENT Y13



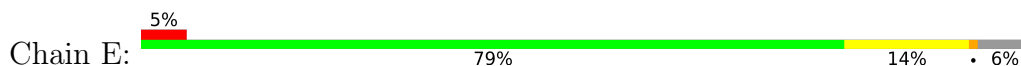
- Molecule 4: PROTEASOME COMPONENT PRE6

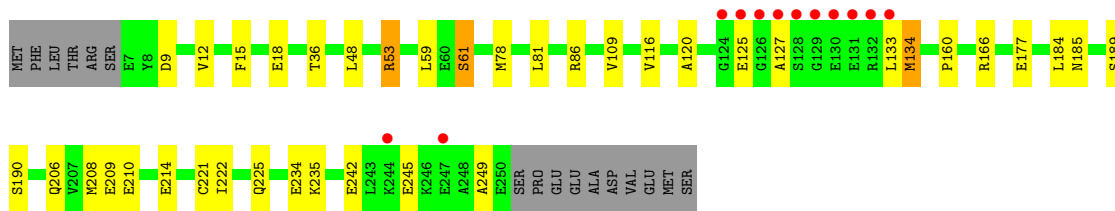


- Molecule 4: PROTEASOME COMPONENT PRE6

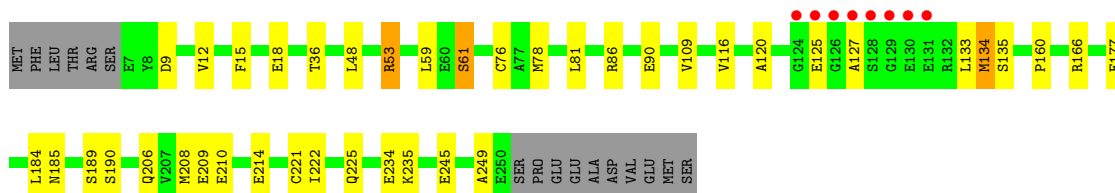
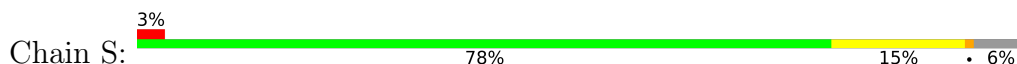


- Molecule 5: PROTEASOME COMPONENT PUP2

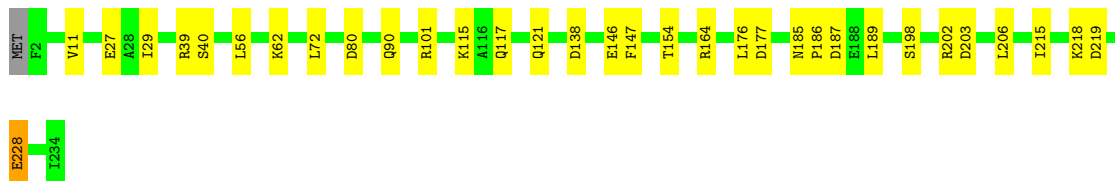
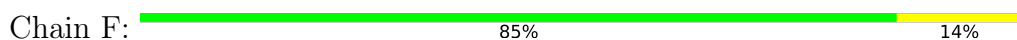




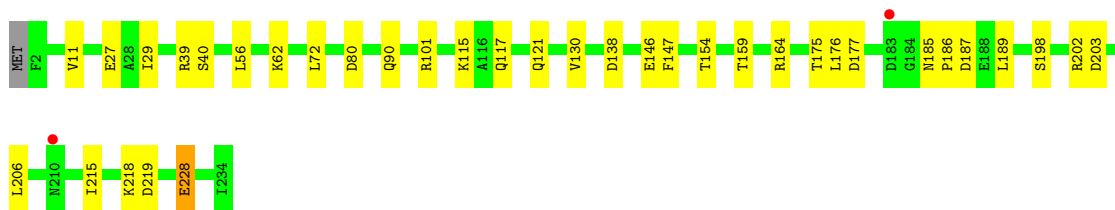
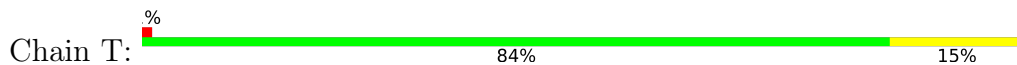
● Molecule 5: PROTEASOME COMPONENT PUP2



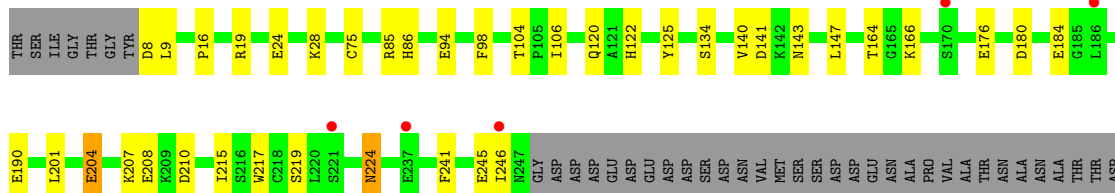
● Molecule 6: PROTEASOME COMPONENT PRE5

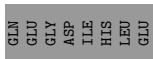


● Molecule 6: PROTEASOME COMPONENT PRE5

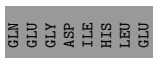
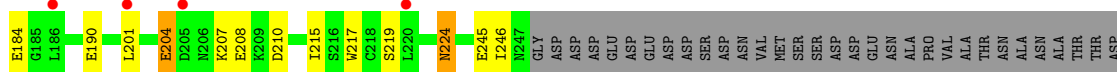


● Molecule 7: PROTEASOME COMPONENT C1

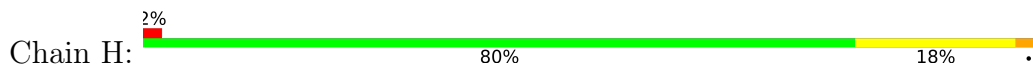




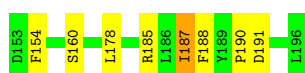
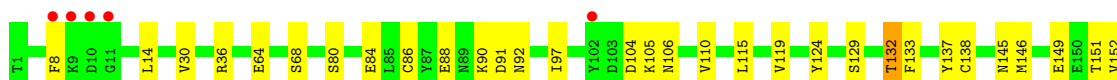
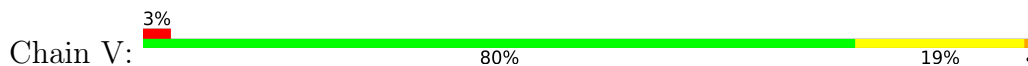
Molecule 7: PROTEASOME COMPONENT C1



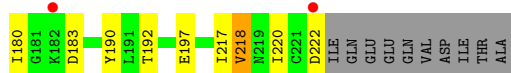
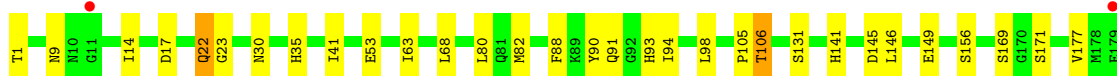
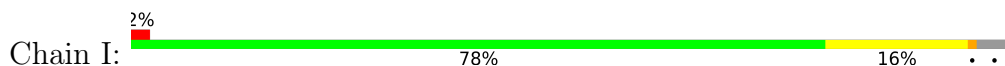
Molecule 8: PROTEASOME COMPONENT PRE3



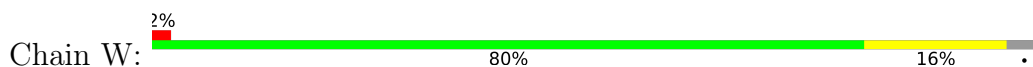
Molecule 8: PROTEASOME COMPONENT PRE3



Molecule 9: PROTEASOME COMPONENT PUP1

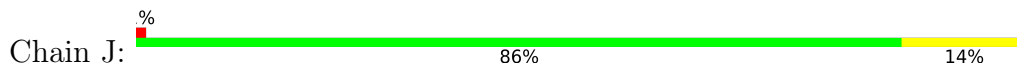


Molecule 9: PROTEASOME COMPONENT PUP1

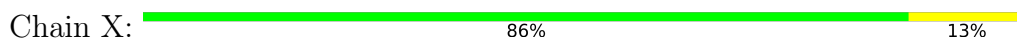




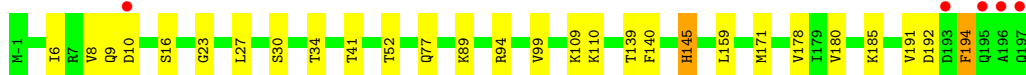
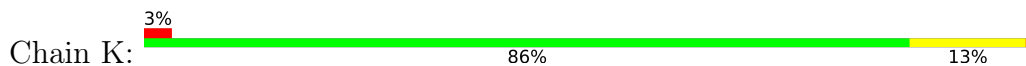
- Molecule 10: PROTEASOME COMPONENT PUP3



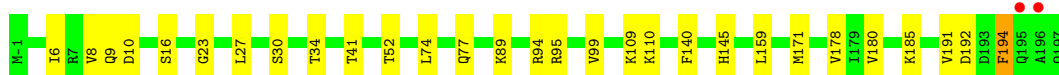
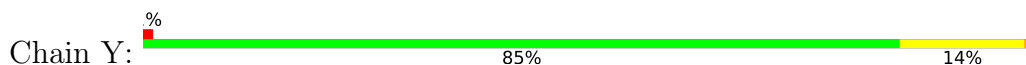
- Molecule 10: PROTEASOME COMPONENT PUP3



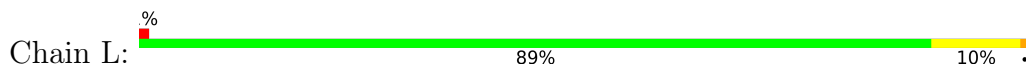
- Molecule 11: PROTEASOME COMPONENT C11



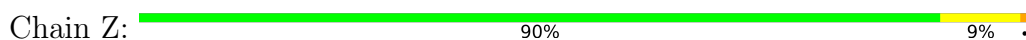
- Molecule 11: PROTEASOME COMPONENT C11




- Molecule 12: PROTEASOME COMPONENT PRE2



- Molecule 12: PROTEASOME COMPONENT PRE2




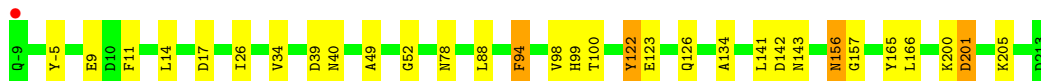
● Molecule 13: PROTEASOME COMPONENT C5

Chain M:  87% 11%




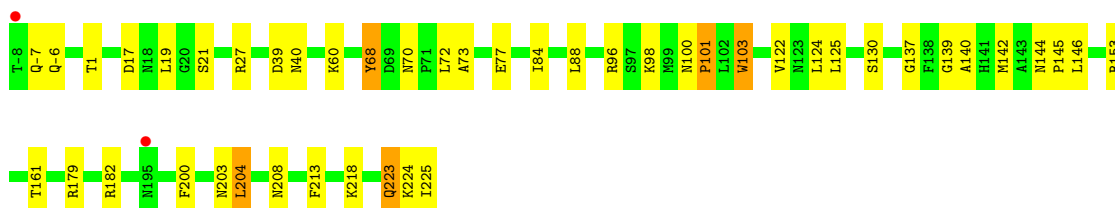
● Molecule 13: PROTEASOME COMPONENT C5

Chain a:  86% 12%




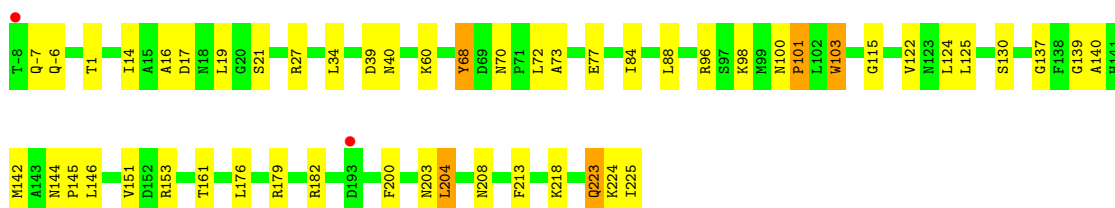
● Molecule 14: PROTEASOME COMPONENT PRE4

Chain N:  80% 18%



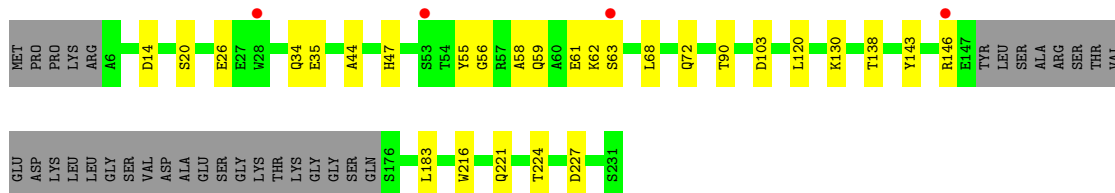
● Molecule 14: PROTEASOME COMPONENT PRE4

Chain b:  78% 20%



● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

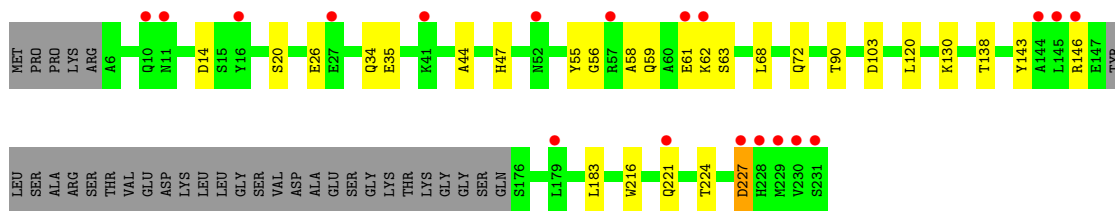
Chain c:  74% 12% 14% 2%



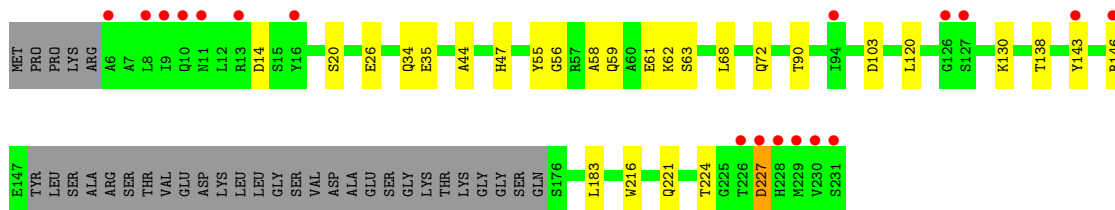
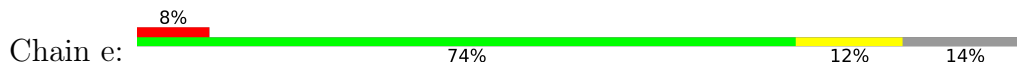
● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

Chain d:  74% 12% 14% 8%

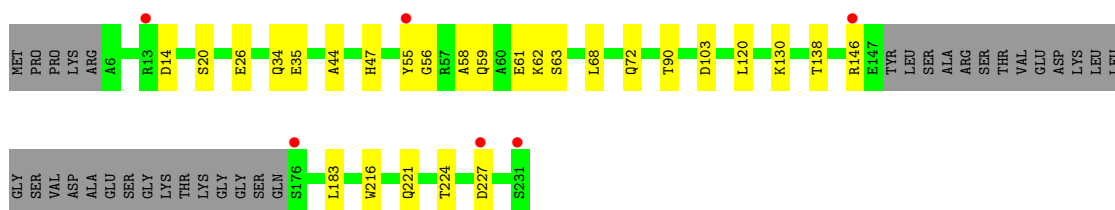
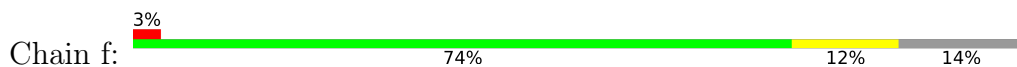




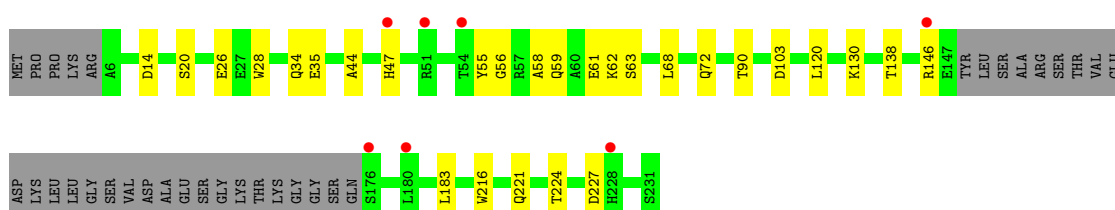
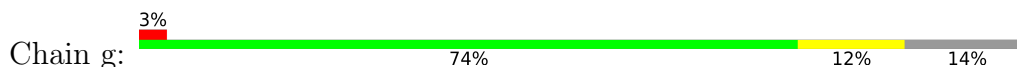
● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



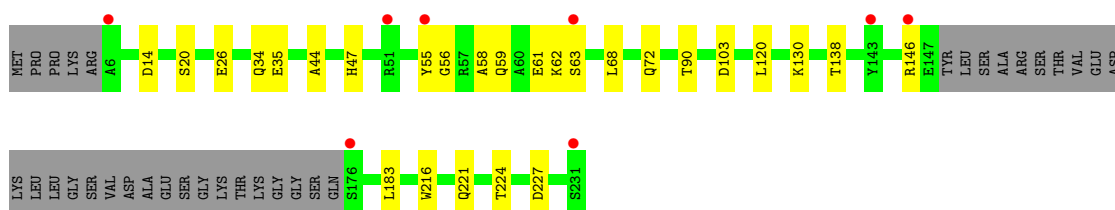
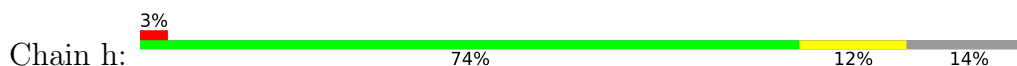
● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



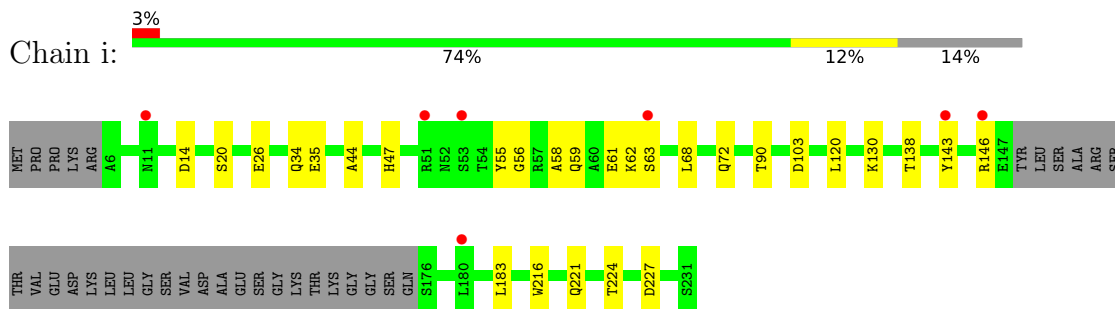
● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



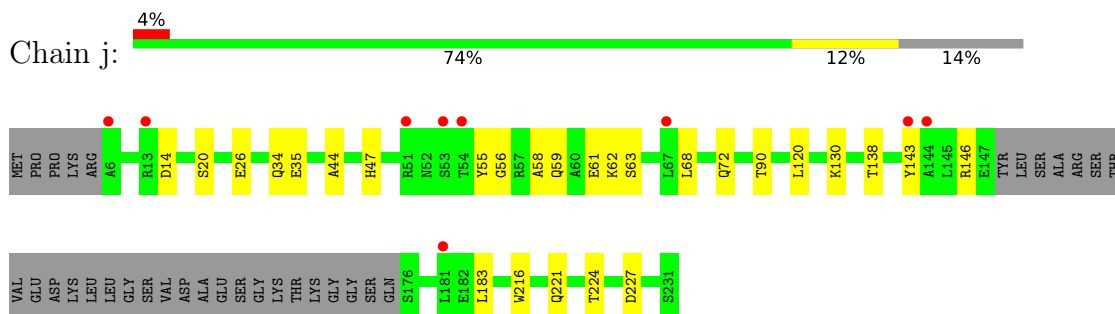
● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



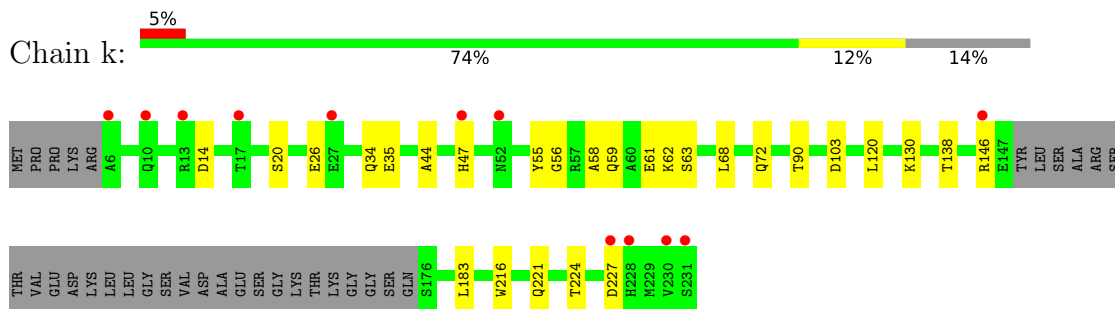
- Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



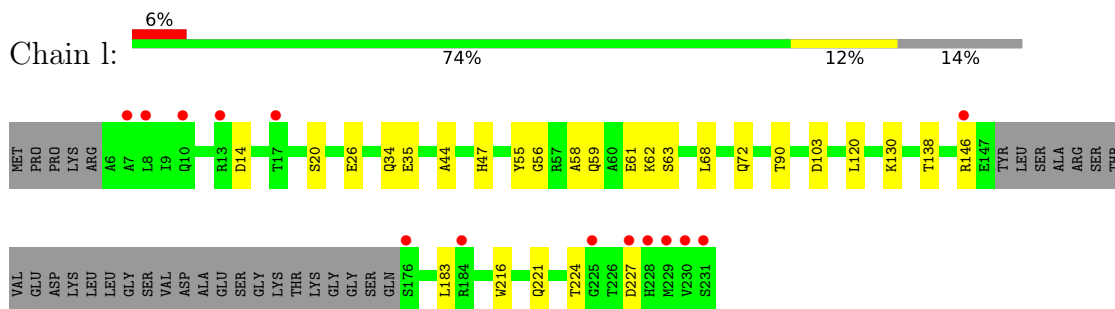
- Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



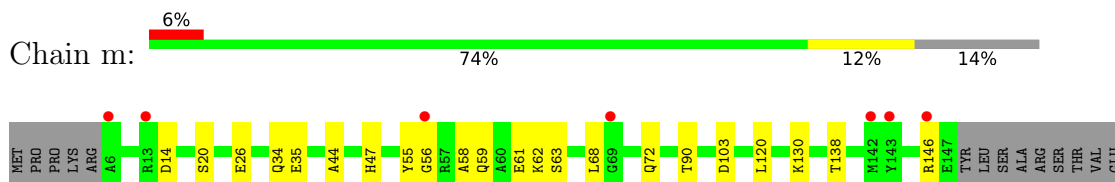
- Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

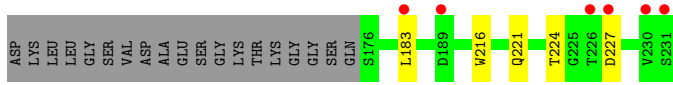


- Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

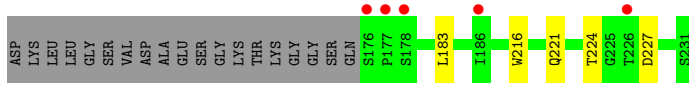
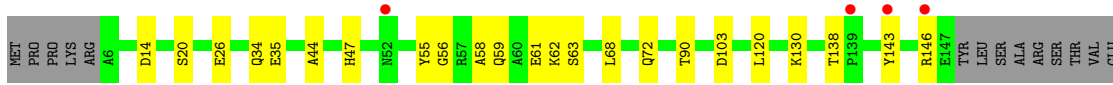
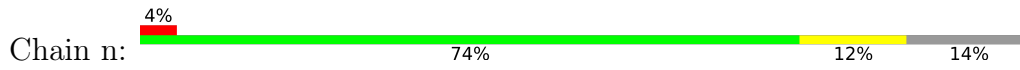


- Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

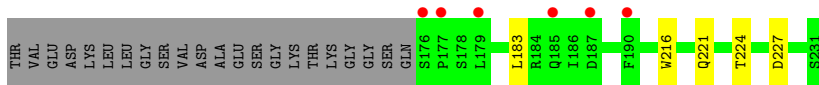
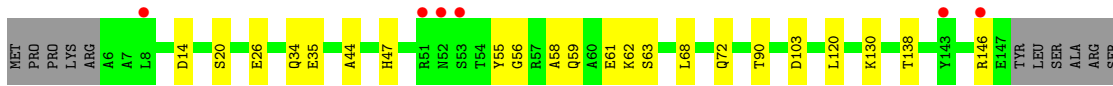
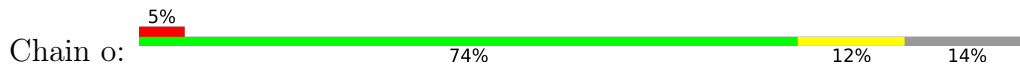




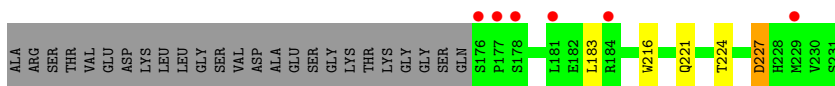
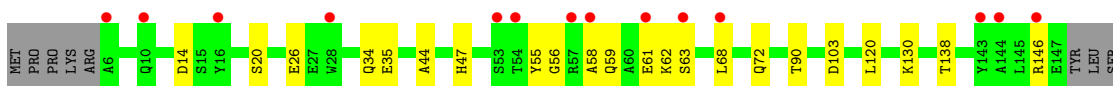
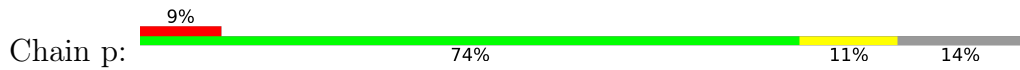
● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



● Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.96Å 232.13Å 296.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 39.84 – 3.22	Depositor EDS
% Data completeness (in resolution range)	86.6 (50.00-3.20) 88.2 (39.84-3.22)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.25Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.255 , 0.325 0.267 , 0.330	Depositor DCC
$R_{free}$ test set	1028 reflections (0.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtrriage
Anisotropy	0.529	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 78.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	70622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: MG

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	A	0.66	0/1918	0.88	1/2597 (0.0%)
1	O	0.63	0/1918	0.88	1/2597 (0.0%)
2	B	0.65	0/1903	0.86	2/2578 (0.1%)
2	P	0.64	0/1903	0.87	1/2578 (0.0%)
3	C	0.66	0/1897	0.88	2/2569 (0.1%)
3	Q	0.68	0/1897	0.88	2/2569 (0.1%)
4	D	0.64	0/1890	0.90	4/2560 (0.2%)
4	R	0.64	0/1890	0.91	5/2560 (0.2%)
5	E	0.68	0/1896	0.84	0/2555
5	S	0.68	1/1896 (0.1%)	0.84	0/2555
6	F	0.59	0/1823	0.82	0/2463
6	T	0.64	0/1823	0.83	0/2463
7	G	0.62	1/1908 (0.1%)	0.80	0/2576
7	U	0.61	0/1908	0.80	0/2576
8	H	0.63	0/1539	0.82	0/2084
8	V	0.62	0/1539	0.81	0/2084
9	I	0.64	1/1715 (0.1%)	0.83	1/2326 (0.0%)
9	W	0.62	0/1715	0.82	0/2326
10	J	0.65	0/1611	0.88	1/2174 (0.0%)
10	X	0.65	0/1611	0.88	1/2174 (0.0%)
11	K	0.70	0/1613	0.84	1/2173 (0.0%)
11	Y	0.68	0/1613	0.84	1/2173 (0.0%)
12	L	0.67	0/1683	0.87	0/2277
12	Z	0.66	0/1683	0.87	0/2277
13	M	0.65	0/1795	0.87	1/2420 (0.0%)
13	a	0.68	0/1795	0.86	1/2420 (0.0%)
14	N	0.63	0/1855	0.88	1/2514 (0.0%)
14	b	0.65	0/1855	0.88	3/2514 (0.1%)
15	c	0.63	0/1551	0.78	1/2099 (0.0%)
15	d	0.64	0/1551	0.79	1/2099 (0.0%)
15	e	0.64	0/1551	0.79	1/2099 (0.0%)
15	f	0.63	0/1551	0.80	1/2099 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
15	g	0.67	1/1551 (0.1%)	0.79	1/2099 (0.0%)
15	h	0.62	0/1551	0.79	1/2099 (0.0%)
15	i	0.62	0/1551	0.80	1/2099 (0.0%)
15	j	0.63	0/1551	0.78	1/2099 (0.0%)
15	k	0.63	0/1551	0.79	1/2099 (0.0%)
15	l	0.63	0/1551	0.79	1/2099 (0.0%)
15	m	0.62	0/1551	0.79	1/2099 (0.0%)
15	n	0.61	0/1551	0.78	1/2099 (0.0%)
15	o	0.61	0/1551	0.79	1/2099 (0.0%)
15	p	0.63	0/1551	0.79	1/2099 (0.0%)
All	All	0.64	4/71806 (0.0%)	0.84	43/97118 (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
3	C	0	1
3	Q	0	1
9	I	0	1
9	W	0	1
13	M	0	1
13	a	0	2
14	N	0	1
14	b	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	76	CYS	CB-SG	-5.85	1.72	1.81
7	G	75	CYS	CB-SG	-5.72	1.72	1.81
9	I	1	THR	CA-CB	5.43	1.67	1.53
15	g	28	TRP	CB-CG	-5.12	1.41	1.50

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	92	GLY	N-CA-C	-7.82	93.56	113.10
10	X	92	GLY	N-CA-C	-7.59	94.13	113.10
4	D	52	LEU	CA-CB-CG	6.98	131.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	52	LEU	CA-CB-CG	6.87	131.10	115.30
4	R	8	LEU	N-CA-C	6.38	128.21	111.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	20	TYR	Sidechain
9	I	190	TYR	Sidechain
13	M	165	TYR	Sidechain
14	N	68	TYR	Sidechain
3	Q	20	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	A	236/252 (94%)	172 (73%)	44 (19%)	20 (8%)	<a href="#">1</a> <a href="#">4</a>
1	O	236/252 (94%)	174 (74%)	42 (18%)	20 (8%)	<a href="#">1</a> <a href="#">4</a>
2	B	245/250 (98%)	170 (69%)	56 (23%)	19 (8%)	<a href="#">1</a> <a href="#">6</a>
2	P	245/250 (98%)	174 (71%)	53 (22%)	18 (7%)	<a href="#">1</a> <a href="#">7</a>
3	C	239/245 (98%)	191 (80%)	29 (12%)	19 (8%)	<a href="#">1</a> <a href="#">6</a>
3	Q	239/245 (98%)	187 (78%)	32 (13%)	20 (8%)	<a href="#">1</a> <a href="#">5</a>
4	D	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	<a href="#">1</a> <a href="#">10</a>
4	R	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	<a href="#">1</a> <a href="#">10</a>
5	E	242/260 (93%)	192 (79%)	36 (15%)	14 (6%)	<a href="#">1</a> <a href="#">13</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	242/260 (93%)	192 (79%)	35 (14%)	15 (6%)	1	11
6	F	231/234 (99%)	189 (82%)	36 (16%)	6 (3%)	5	31
6	T	231/234 (99%)	190 (82%)	32 (14%)	9 (4%)	3	22
7	G	238/287 (83%)	193 (81%)	37 (16%)	8 (3%)	3	24
7	U	238/287 (83%)	194 (82%)	34 (14%)	10 (4%)	3	20
8	H	194/196 (99%)	148 (76%)	30 (16%)	16 (8%)	1	5
8	V	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	1	9
9	I	220/232 (95%)	178 (81%)	27 (12%)	15 (7%)	1	9
9	W	220/232 (95%)	176 (80%)	31 (14%)	13 (6%)	1	12
10	J	202/205 (98%)	165 (82%)	33 (16%)	4 (2%)	7	38
10	X	202/205 (98%)	168 (83%)	30 (15%)	4 (2%)	7	38
11	K	196/198 (99%)	163 (83%)	24 (12%)	9 (5%)	2	18
11	Y	196/198 (99%)	160 (82%)	28 (14%)	8 (4%)	3	21
12	L	210/212 (99%)	180 (86%)	27 (13%)	3 (1%)	11	46
12	Z	210/212 (99%)	178 (85%)	29 (14%)	3 (1%)	11	46
13	M	220/222 (99%)	188 (86%)	24 (11%)	8 (4%)	3	23
13	a	220/222 (99%)	186 (84%)	25 (11%)	9 (4%)	3	21
14	N	231/233 (99%)	169 (73%)	43 (19%)	19 (8%)	1	5
14	b	231/233 (99%)	170 (74%)	40 (17%)	21 (9%)	1	3
15	c	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	15
15	d	194/231 (84%)	162 (84%)	21 (11%)	11 (6%)	1	14
15	e	194/231 (84%)	161 (83%)	22 (11%)	11 (6%)	1	14
15	f	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	15
15	g	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	15
15	h	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	15
15	i	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	15
15	j	194/231 (84%)	162 (84%)	23 (12%)	9 (5%)	2	18
15	k	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	2	15
15	l	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	2	15
15	m	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	2	15
15	n	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	o	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	2	15
15	p	194/231 (84%)	163 (84%)	20 (10%)	11 (6%)	1	14
All	All	8998/9794 (92%)	7221 (80%)	1282 (14%)	495 (6%)	2	14

5 of 495 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	19	PHE
1	A	60	PRO
1	A	115	ASP
1	A	221	ASN

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/210 (97%)	173 (85%)	31 (15%)	3	13
1	O	204/210 (97%)	174 (85%)	30 (15%)	3	14
2	B	200/209 (96%)	169 (84%)	31 (16%)	2	12
2	P	200/209 (96%)	167 (84%)	33 (16%)	2	10
3	C	198/204 (97%)	168 (85%)	30 (15%)	3	13
3	Q	198/204 (97%)	169 (85%)	29 (15%)	3	15
4	D	209/226 (92%)	175 (84%)	34 (16%)	2	11
4	R	209/226 (92%)	176 (84%)	33 (16%)	2	12
5	E	198/215 (92%)	170 (86%)	28 (14%)	3	16
5	S	198/215 (92%)	170 (86%)	28 (14%)	3	16
6	F	192/193 (100%)	164 (85%)	28 (15%)	3	15
6	T	192/193 (100%)	164 (85%)	28 (15%)	3	15
7	G	199/238 (84%)	167 (84%)	32 (16%)	2	11
7	U	199/238 (84%)	165 (83%)	34 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	161/162 (99%)	132 (82%)	29 (18%)	1	9
8	V	161/162 (99%)	133 (83%)	28 (17%)	2	10
9	I	181/190 (95%)	156 (86%)	25 (14%)	3	16
9	W	181/190 (95%)	157 (87%)	24 (13%)	4	18
10	J	172/173 (99%)	149 (87%)	23 (13%)	4	18
10	X	172/173 (99%)	150 (87%)	22 (13%)	4	20
11	K	175/175 (100%)	155 (89%)	20 (11%)	5	24
11	Y	175/175 (100%)	154 (88%)	21 (12%)	5	22
12	L	169/169 (100%)	147 (87%)	22 (13%)	4	19
12	Z	169/169 (100%)	148 (88%)	21 (12%)	4	21
13	M	185/185 (100%)	163 (88%)	22 (12%)	5	22
13	a	185/185 (100%)	162 (88%)	23 (12%)	4	21
14	N	199/199 (100%)	169 (85%)	30 (15%)	3	14
14	b	199/199 (100%)	167 (84%)	32 (16%)	2	11
15	c	163/190 (86%)	146 (90%)	17 (10%)	7	28
15	d	163/190 (86%)	146 (90%)	17 (10%)	7	28
15	e	163/190 (86%)	146 (90%)	17 (10%)	7	28
15	f	163/190 (86%)	147 (90%)	16 (10%)	8	31
15	g	163/190 (86%)	147 (90%)	16 (10%)	8	31
15	h	163/190 (86%)	147 (90%)	16 (10%)	8	31
15	i	163/190 (86%)	146 (90%)	17 (10%)	7	28
15	j	163/190 (86%)	146 (90%)	17 (10%)	7	28
15	k	163/190 (86%)	147 (90%)	16 (10%)	8	31
15	l	163/190 (86%)	147 (90%)	16 (10%)	8	31
15	m	163/190 (86%)	147 (90%)	16 (10%)	8	31
15	n	163/190 (86%)	146 (90%)	17 (10%)	7	28
15	o	163/190 (86%)	147 (90%)	16 (10%)	8	31
15	p	163/190 (86%)	147 (90%)	16 (10%)	8	31
All	All	7566/8156 (93%)	6565 (87%)	1001 (13%)	4	19

5 of 1001 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	140	TYR
15	i	227	ASP
7	U	86	HIS
15	i	68	LEU
15	m	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 268 such sidechains are listed below:

Mol	Chain	Res	Type
15	j	80	ASN
15	l	52	ASN
15	o	99	HIS
1	O	126	GLN
1	O	39	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	238/252 (94%)	0.12	8 (3%) 45 29	45, 88, 99, 100	0
1	O	238/252 (94%)	0.11	6 (2%) 57 43	51, 89, 99, 100	0
2	B	247/250 (98%)	0.04	4 (1%) 72 59	39, 78, 96, 100	0
2	P	247/250 (98%)	-0.07	2 (0%) 86 78	46, 81, 98, 100	0
3	C	241/245 (98%)	-0.09	4 (1%) 70 57	35, 71, 99, 100	0
3	Q	241/245 (98%)	0.01	9 (3%) 41 26	37, 77, 99, 100	0
4	D	239/254 (94%)	-0.08	5 (2%) 63 49	34, 68, 98, 100	0
4	R	239/254 (94%)	-0.09	5 (2%) 63 49	37, 74, 99, 100	0
5	E	244/260 (93%)	-0.04	12 (4%) 29 17	29, 67, 98, 100	0
5	S	244/260 (93%)	0.01	8 (3%) 46 30	41, 72, 99, 100	0
6	F	233/234 (99%)	-0.25	0 100 100	33, 69, 87, 98	0
6	T	233/234 (99%)	-0.06	2 (0%) 84 75	45, 74, 92, 100	0
7	G	240/287 (83%)	0.08	5 (2%) 63 49	45, 82, 98, 100	0
7	U	240/287 (83%)	0.17	5 (2%) 63 49	52, 85, 99, 100	0
8	H	196/196 (100%)	-0.07	3 (1%) 73 61	51, 79, 97, 100	0
8	V	196/196 (100%)	0.02	5 (2%) 56 40	56, 81, 98, 100	0
9	I	222/232 (95%)	-0.16	4 (1%) 68 55	44, 74, 95, 100	0
9	W	222/232 (95%)	-0.10	5 (2%) 60 47	44, 75, 93, 100	0
10	J	204/205 (99%)	-0.36	3 (1%) 73 61	29, 60, 85, 100	0
10	X	204/205 (99%)	-0.41	1 (0%) 91 86	33, 60, 82, 95	0
11	K	198/198 (100%)	-0.27	5 (2%) 57 43	23, 52, 80, 100	0
11	Y	198/198 (100%)	-0.35	2 (1%) 82 72	30, 56, 84, 100	0
12	L	212/212 (100%)	-0.41	2 (0%) 84 75	30, 52, 72, 96	0
12	Z	212/212 (100%)	-0.53	0 100 100	31, 52, 76, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	222/222 (100%)	-0.35	1 (0%) 91 86	28, 60, 79, 97	0
13	a	222/222 (100%)	-0.31	1 (0%) 91 86	30, 61, 85, 99	0
14	N	233/233 (100%)	-0.15	2 (0%) 84 75	37, 72, 95, 99	0
14	b	233/233 (100%)	-0.08	2 (0%) 84 75	39, 74, 96, 100	0
15	c	198/231 (85%)	0.25	4 (2%) 65 51	58, 90, 99, 100	0
15	d	198/231 (85%)	0.43	19 (9%) 8 4	65, 92, 100, 100	0
15	e	198/231 (85%)	0.40	18 (9%) 9 5	58, 91, 100, 100	0
15	f	198/231 (85%)	0.15	6 (3%) 50 34	47, 89, 99, 100	0
15	g	198/231 (85%)	0.14	7 (3%) 44 28	48, 88, 99, 100	0
15	h	198/231 (85%)	0.26	8 (4%) 38 25	57, 86, 99, 100	0
15	i	198/231 (85%)	0.25	7 (3%) 44 28	56, 91, 100, 100	0
15	j	198/231 (85%)	0.37	9 (4%) 33 21	60, 94, 100, 100	0
15	k	198/231 (85%)	0.35	12 (6%) 21 12	65, 94, 100, 100	0
15	l	198/231 (85%)	0.29	14 (7%) 16 9	56, 93, 100, 100	0
15	m	198/231 (85%)	0.27	13 (6%) 18 11	56, 94, 100, 100	0
15	n	198/231 (85%)	0.30	9 (4%) 33 21	64, 94, 100, 100	0
15	o	198/231 (85%)	0.40	12 (6%) 21 12	70, 93, 100, 100	0
15	p	198/231 (85%)	0.48	20 (10%) 7 4	67, 95, 100, 100	0
All	All	9110/9794 (93%)	0.01	269 (2%) 50 34	23, 79, 99, 100	0

The worst 5 of 269 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	S	129	GLY	6.4
3	Q	245	THR	6.2
15	k	231	SER	5.7
5	E	127	ALA	5.3
5	S	126	GLY	5.3

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
16	MG	H	1002	1/1	0.73	0.39	81,81,81,81	0
16	MG	U	1014	1/1	0.77	0.30	65,65,65,65	0
16	MG	X	1012	1/1	0.83	0.29	56,56,56,56	0
16	MG	X	1013	1/1	0.87	0.23	79,79,79,79	0
16	MG	I	1001	1/1	0.88	0.16	67,67,67,67	0
16	MG	L	1003	1/1	0.89	0.22	43,43,43,43	0
16	MG	V	1009	1/1	0.89	0.18	39,39,39,39	0
16	MG	G	1007	1/1	0.91	0.10	38,38,38,38	0
16	MG	J	1006	1/1	0.92	0.09	24,24,24,24	0
16	MG	W	1008	1/1	0.95	0.08	67,67,67,67	0
16	MG	J	1005	1/1	0.97	0.26	37,37,37,37	0
16	MG	a	1011	1/1	0.97	0.06	49,49,49,49	0
16	MG	Z	1010	1/1	0.98	0.08	38,38,38,38	0
16	MG	M	1004	1/1	0.98	0.07	26,26,26,26	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.