



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:41 PM GMT

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

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

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

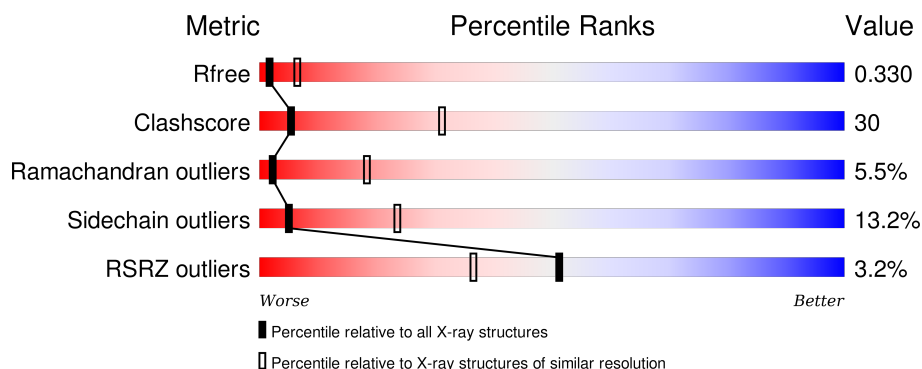
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	 3% 34% 46% 14% • 6%
1	O	252	 3% 32% 47% 14% • 6%
2	B	250	 2% 43% 45% 10% ••
2	P	250	 % 44% 45% 9% ••
3	C	245	 2% 44% 42% 12% •





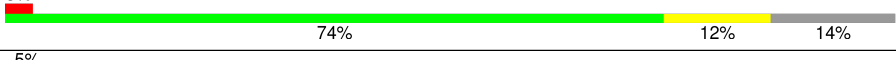
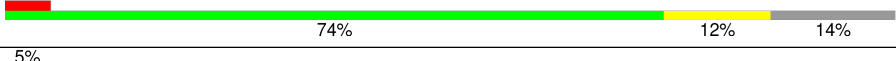
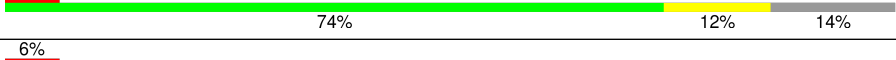
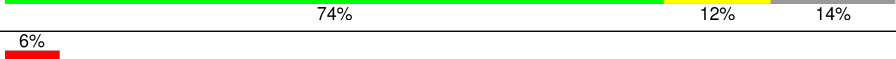


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	245	
4	D	254	
4	R	254	
5	E	260	
5	S	260	
6	F	234	
6	T	234	
7	G	287	
7	U	287	
8	H	196	
8	V	196	
9	I	232	
9	W	232	
10	J	205	
10	X	205	
11	K	198	
11	Y	198	
12	L	212	
12	Z	212	
13	M	222	
13	a	222	
14	N	233	
14	b	233	
15	c	231	
15	d	231	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	e	231	
15	f	231	
15	g	231	
15	h	231	
15	i	231	
15	j	231	
15	k	231	
15	l	231	
15	m	231	
15	n	231	
15	o	231	
15	p	231	

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
16	MG	H	1002	-	-	-	X
16	MG	J	1005	-	-	-	X
16	MG	X	1012	-	-	-	X

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
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
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
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
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			

Continued on next page...

Continued from previous page...

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	UNP P30656
Z	33	ARG	LYS	ENGINEERED	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
15	c	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	d	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	e	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	f	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	g	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	h	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	i	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	j	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	k	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	l	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	m	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	n	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	o	198	Total 1529	C 960	N 267	O 296	S 6	0	0	0
15	p	198	Total 1529	C 960	N 267	O 296	S 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

Continued on next page...

Continued from previous page...

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

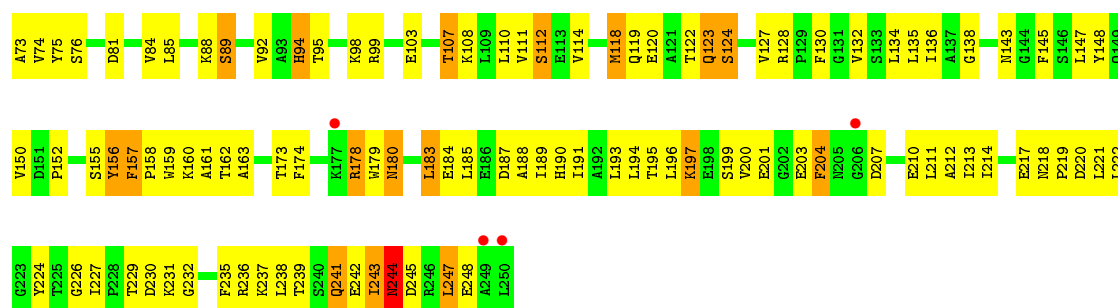
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

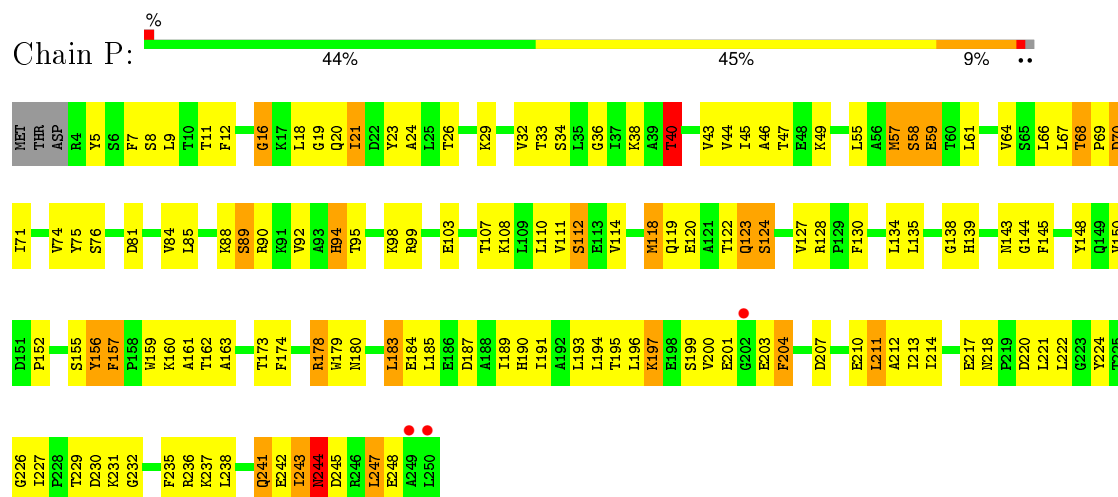
Continued on next page...

Continued from previous page...

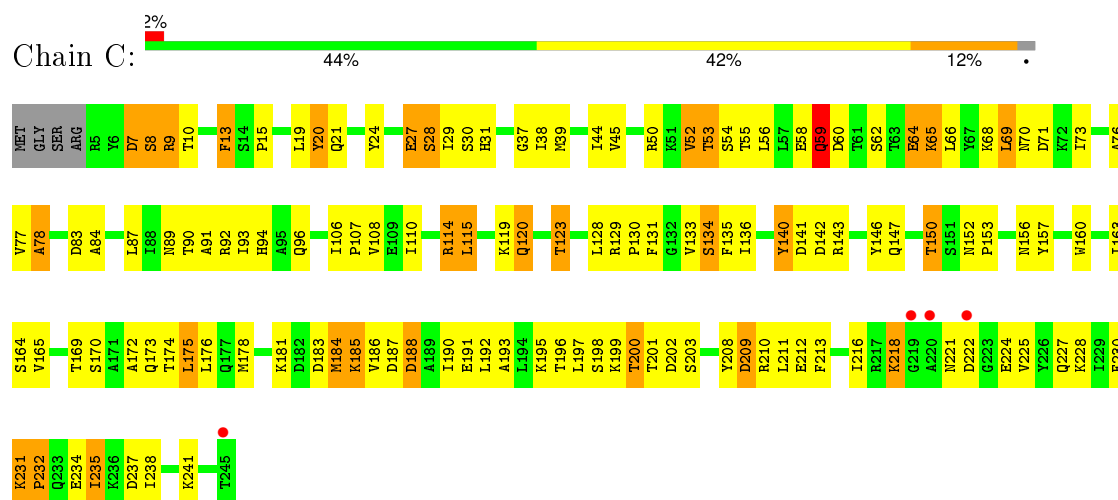
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	M	1	Total	Mg	0	0
			1	1		



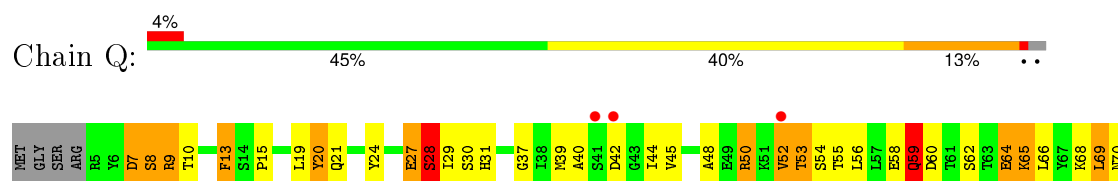
• Molecule 2: PROTEASOME COMPONENT Y7

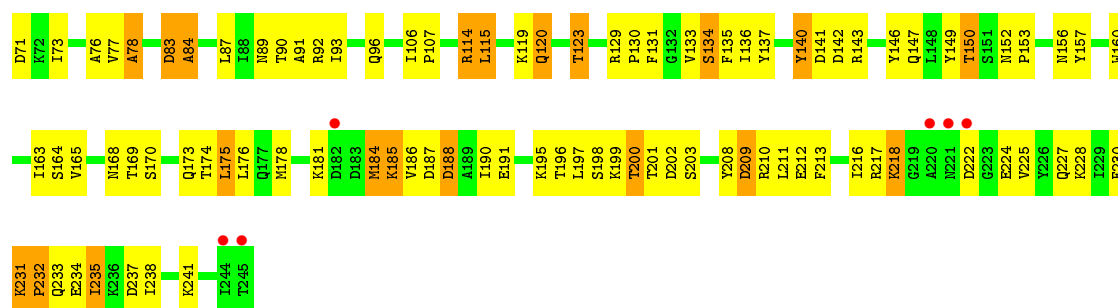


• Molecule 3: PROTEASOME COMPONENT Y13

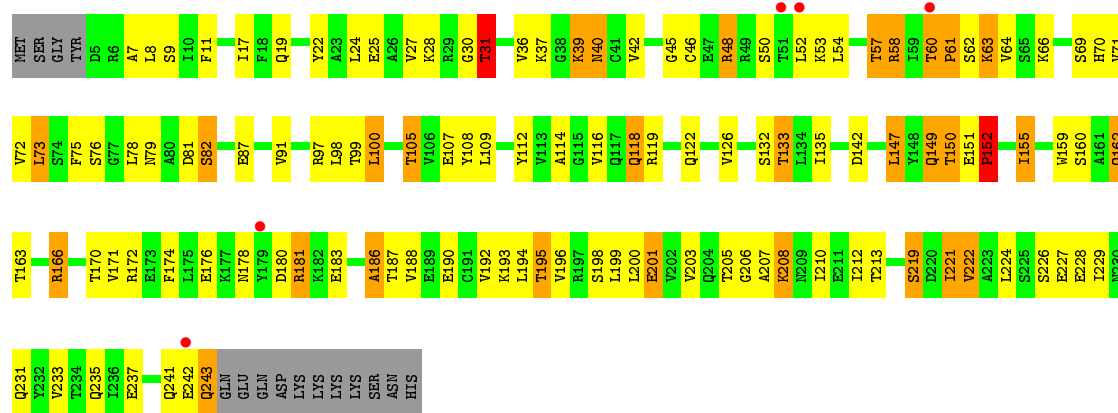


• Molecule 3: PROTEASOME COMPONENT Y13

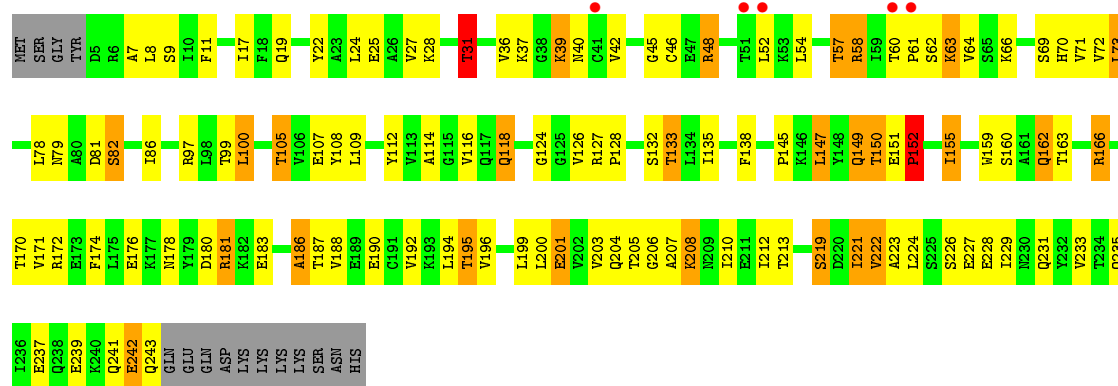




• Molecule 4: PROTEASOME COMPONENT PRE6

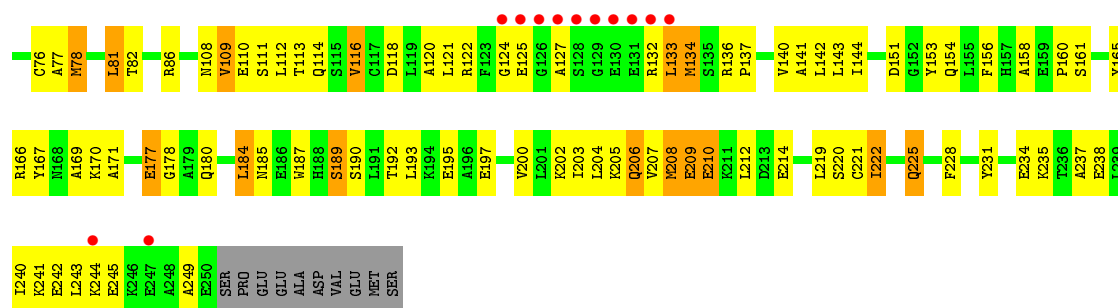


• Molecule 4: PROTEASOME COMPONENT PRE6

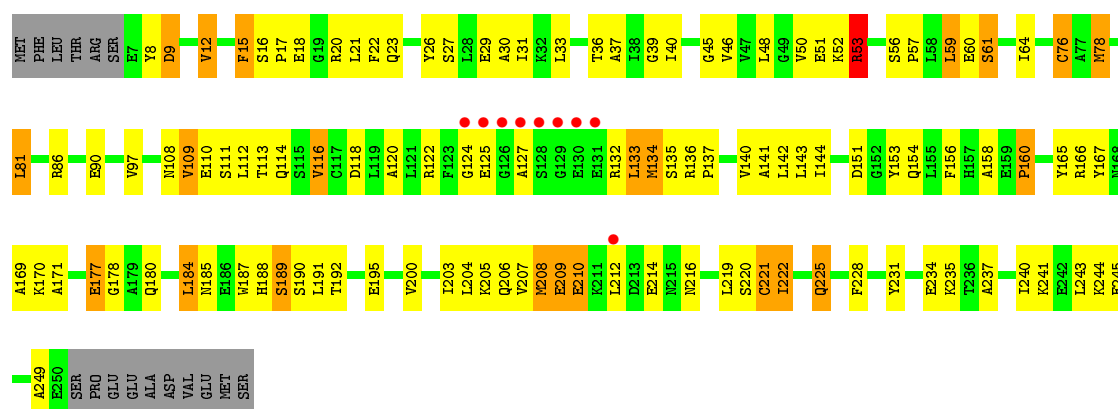


• Molecule 5: PROTEASOME COMPONENT PUP2

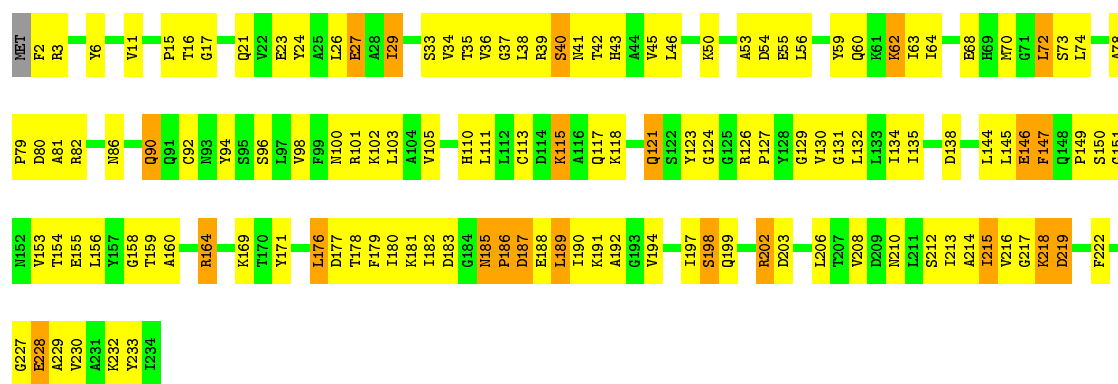




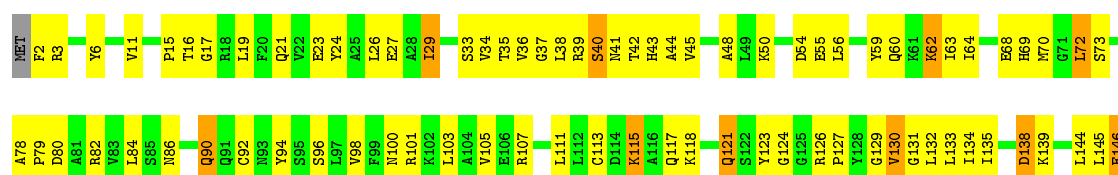
• Molecule 5: PROTEASOME COMPONENT PUP2

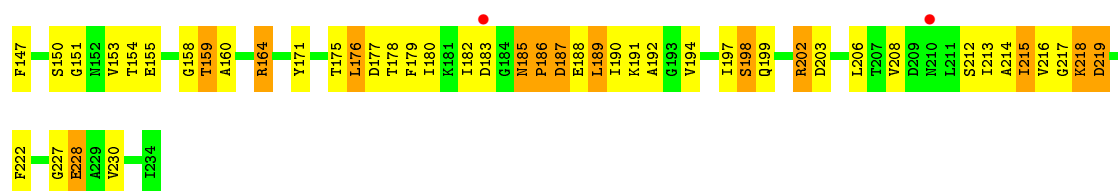


• Molecule 6: PROTEASOME COMPONENT PRE5

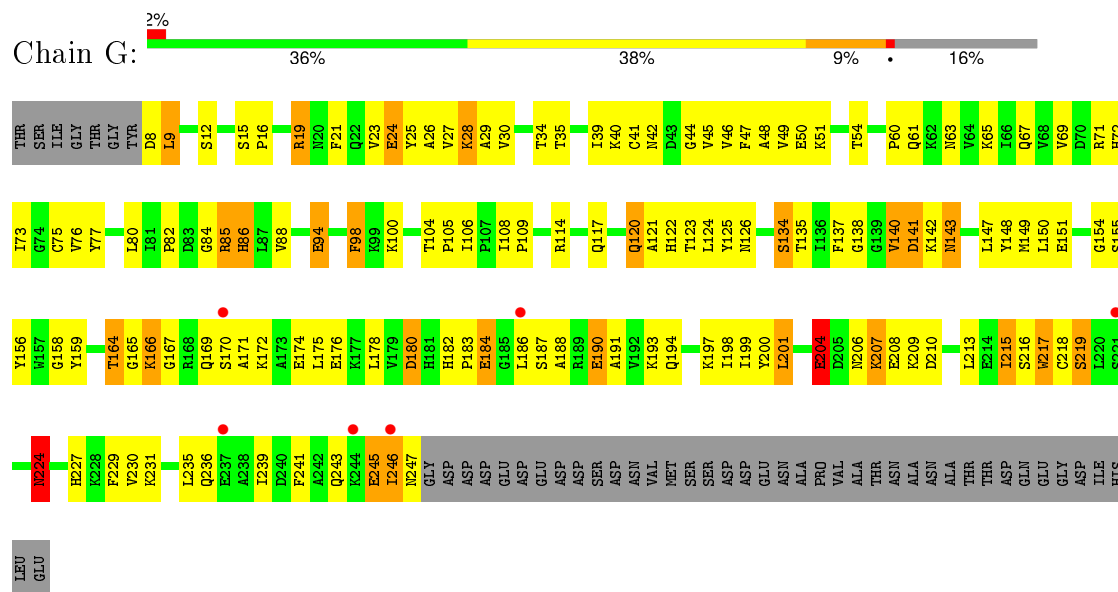


• Molecule 6: PROTEASOME COMPONENT PRE5

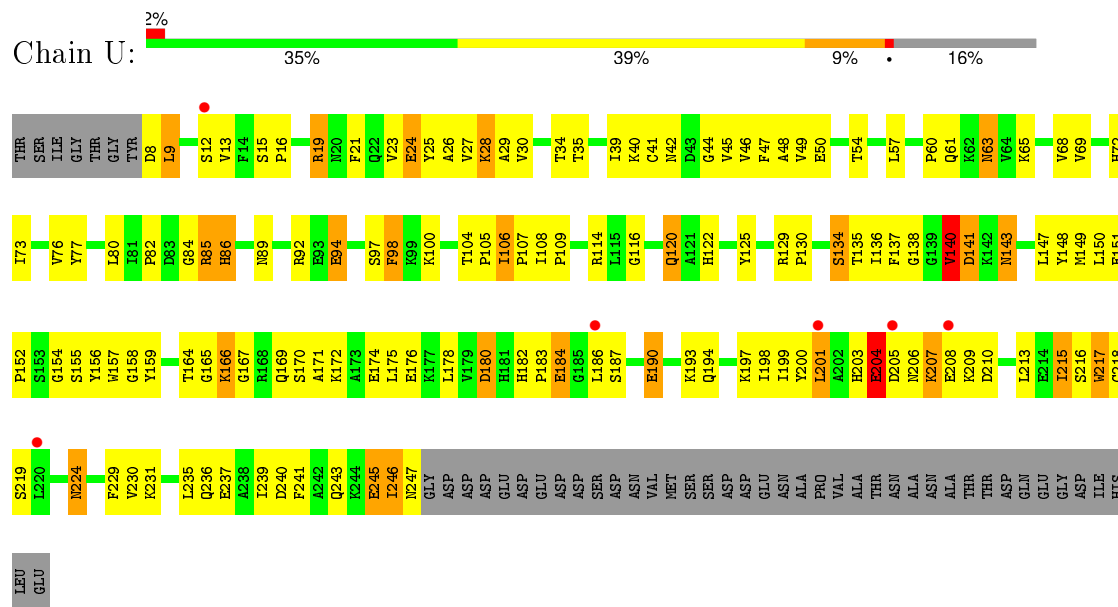




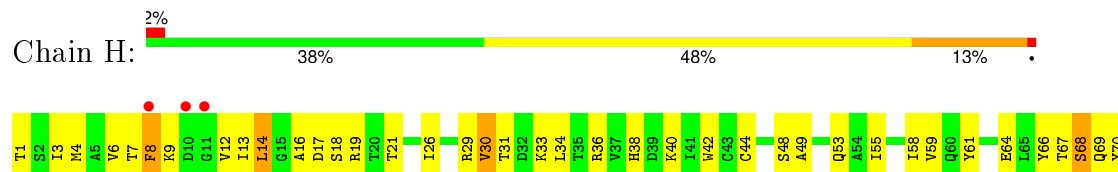
• Molecule 7: PROTEASOME COMPONENT C1

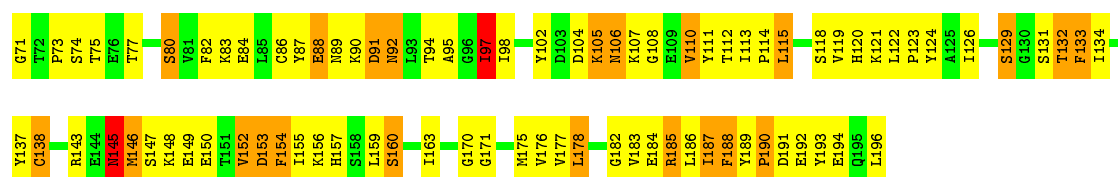


• Molecule 7: PROTEASOME COMPONENT C1

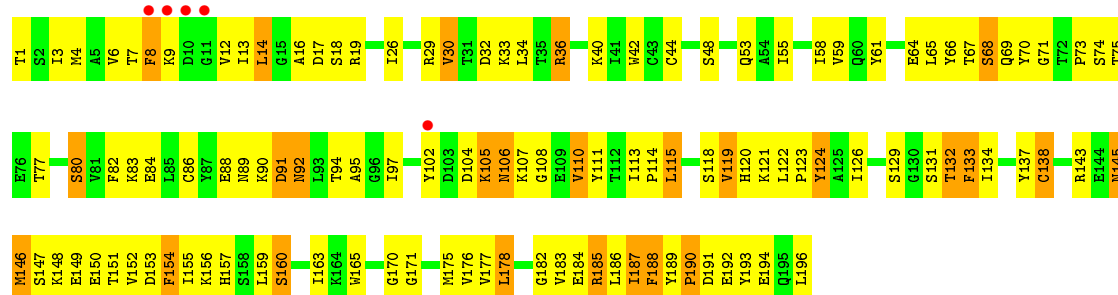
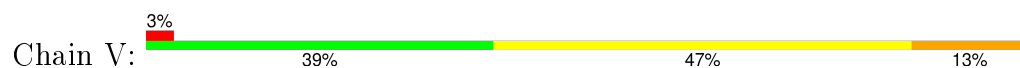


• Molecule 8: PROTEASOME COMPONENT PRE3

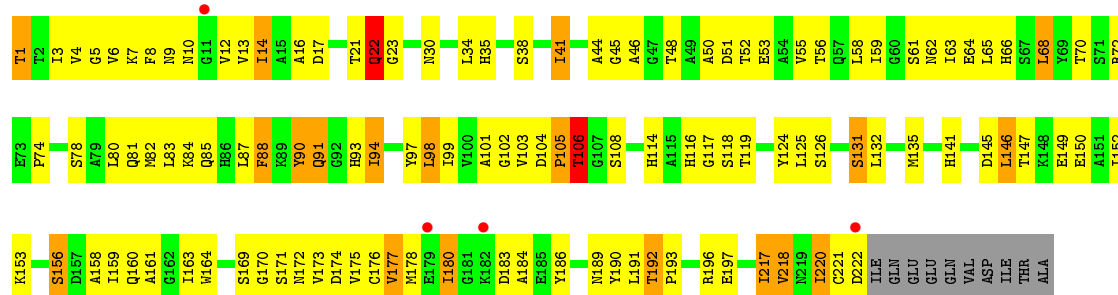
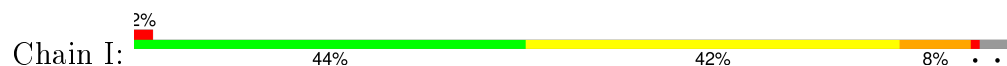




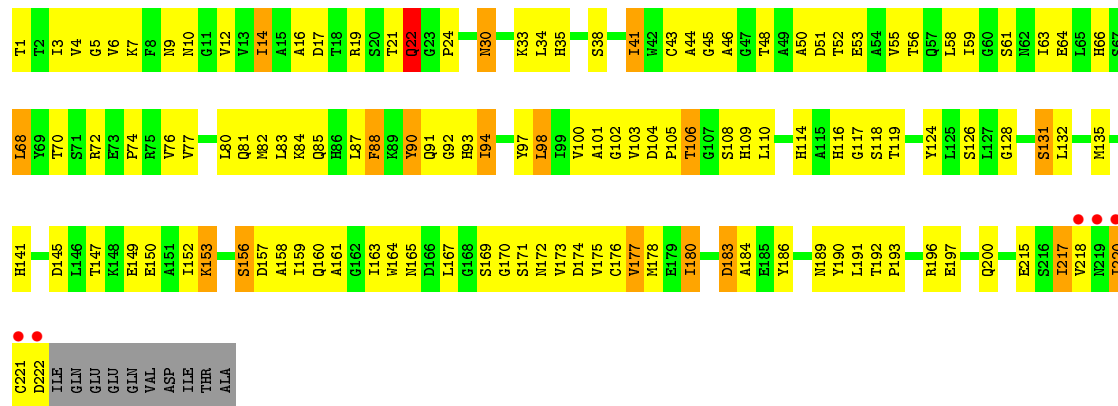
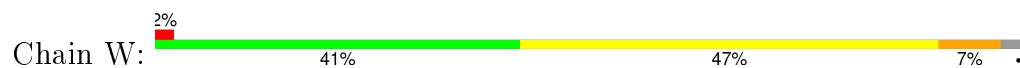
• Molecule 8: PROTEASOME COMPONENT PRE3



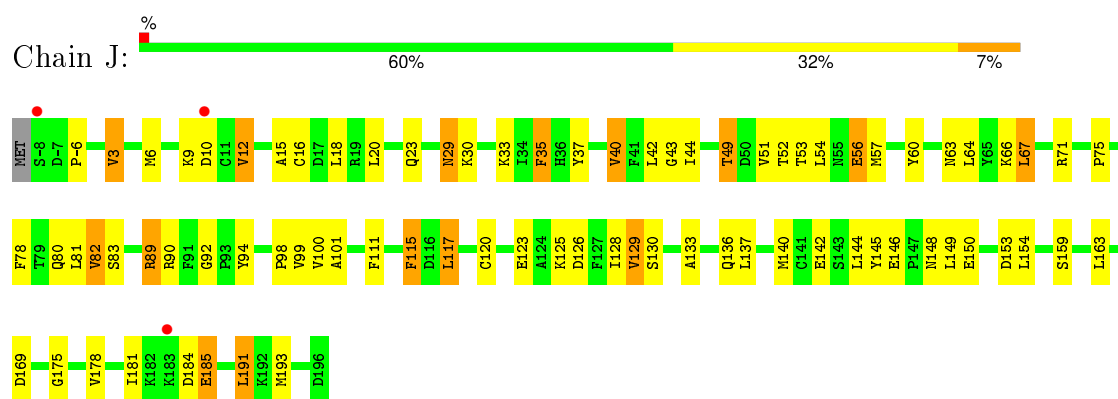
• Molecule 9: PROTEASOME COMPONENT PUP1



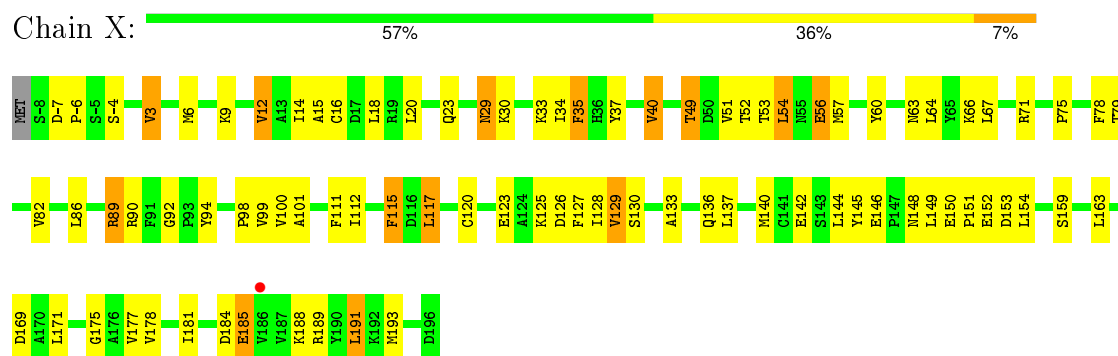
• Molecule 9: PROTEASOME COMPONENT PUP1



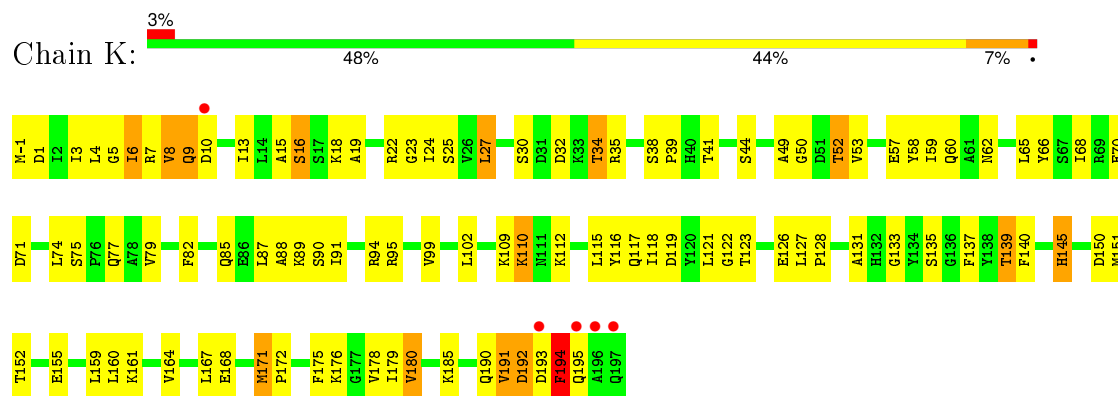
• Molecule 10: PROTEASOME COMPONENT PUP3



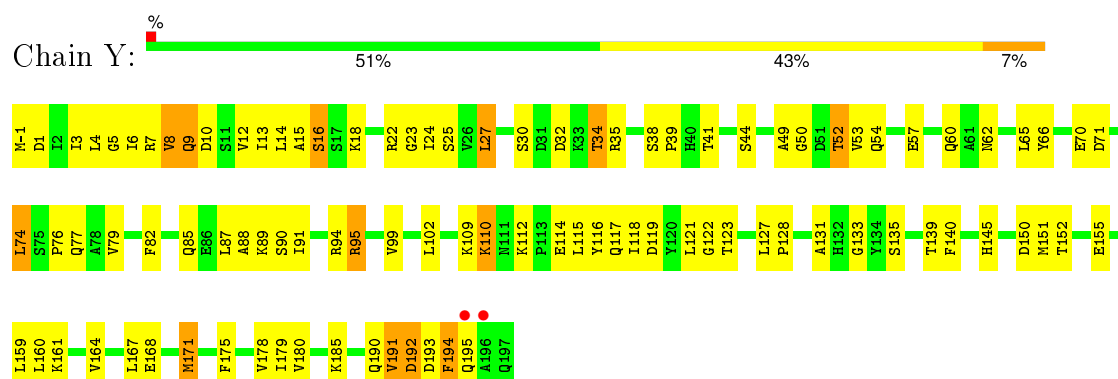
• Molecule 10: PROTEASOME COMPONENT PUP3



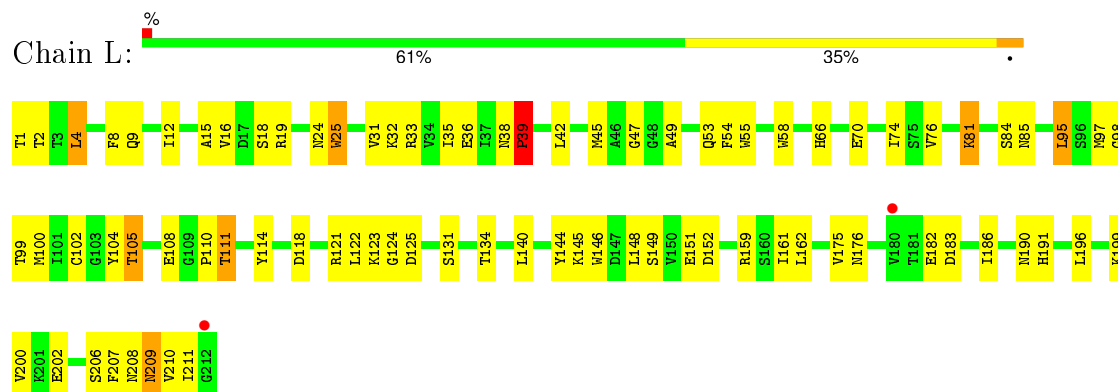
• Molecule 11: PROTEASOME COMPONENT C11



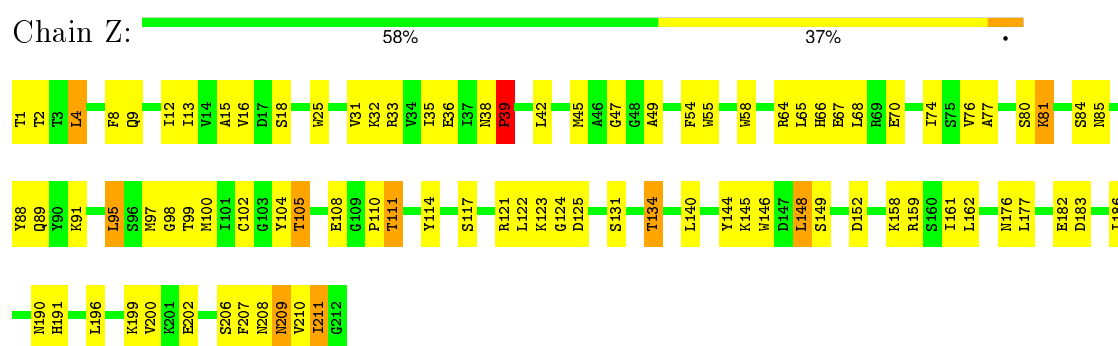
• Molecule 11: PROTEASOME COMPONENT C11



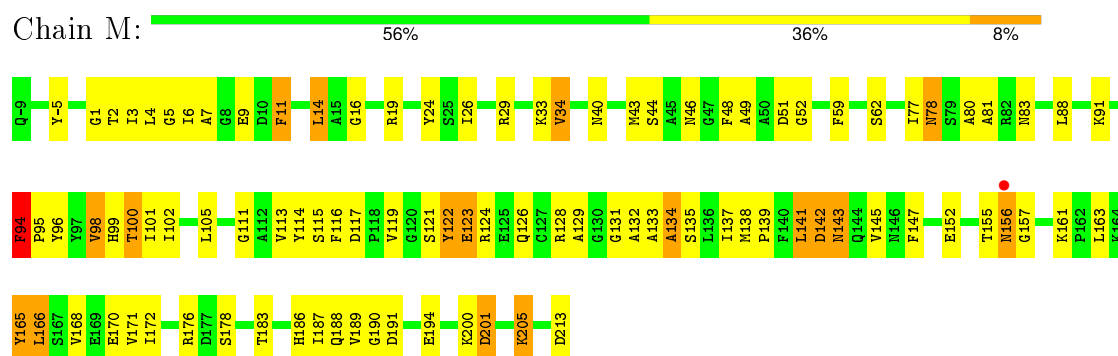
- Molecule 12: PROTEASOME COMPONENT PRE2



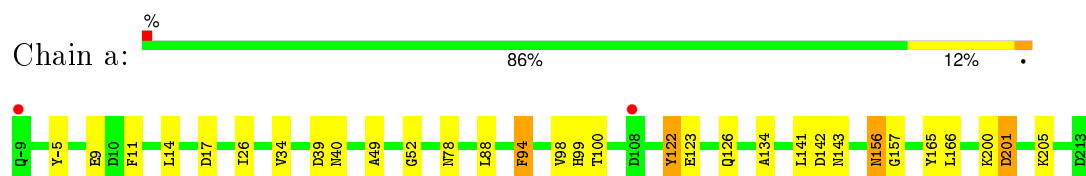
- Molecule 12: PROTEASOME COMPONENT PRE2



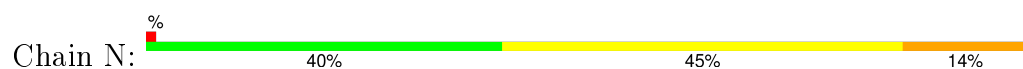
- Molecule 13: PROTEASOME COMPONENT C5

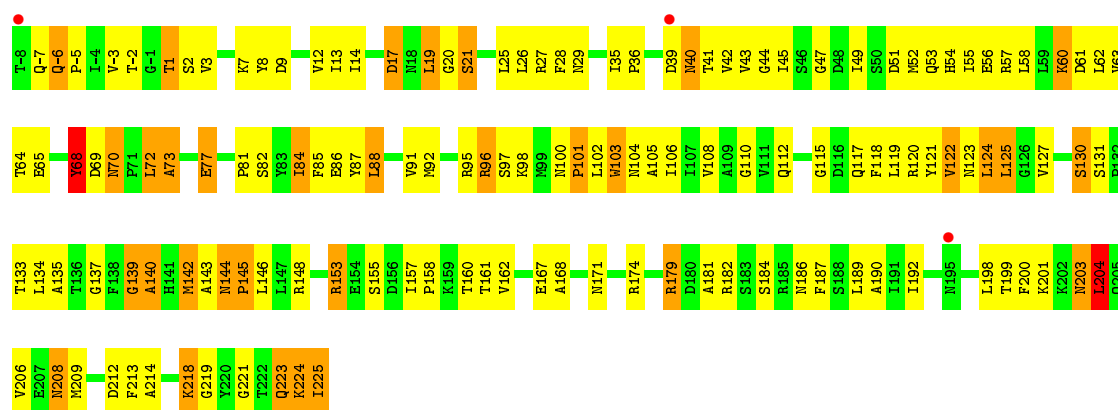


- Molecule 13: PROTEASOME COMPONENT C5

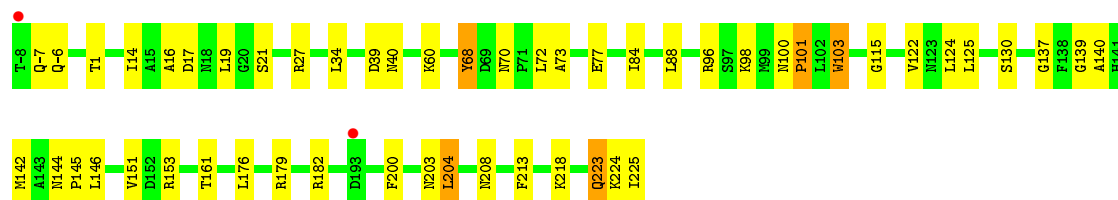
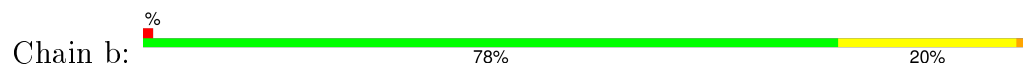


- Molecule 14: PROTEASOME COMPONENT PRE4

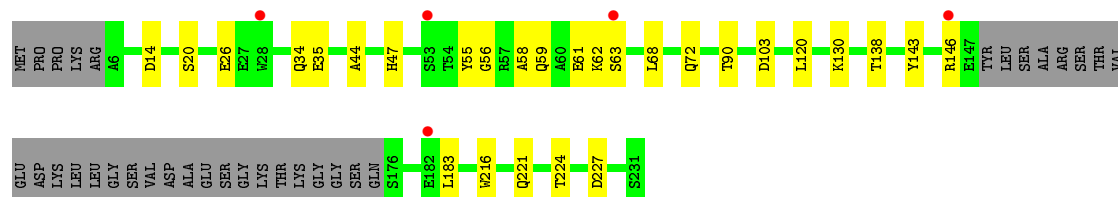
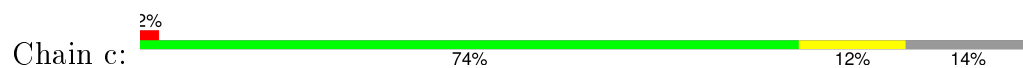




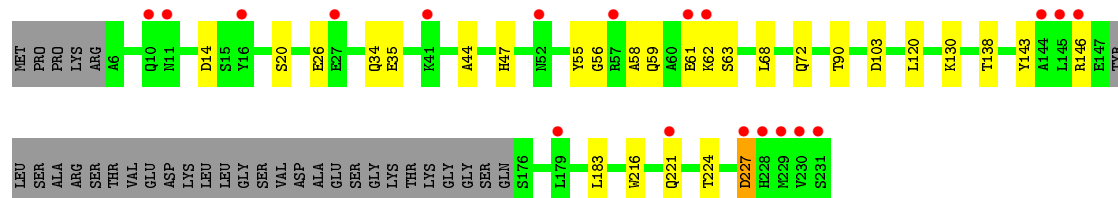
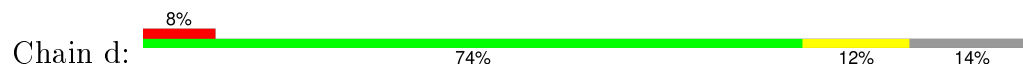
• Molecule 14: PROTEASOME COMPONENT PRE4



• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

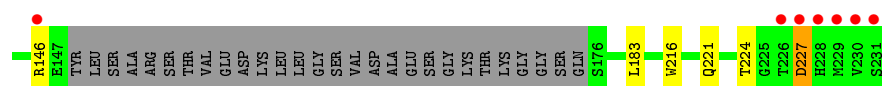


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

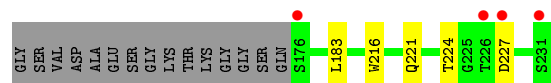
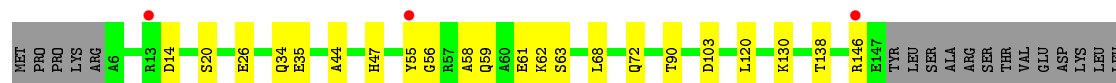


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

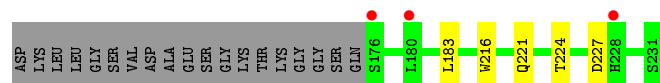
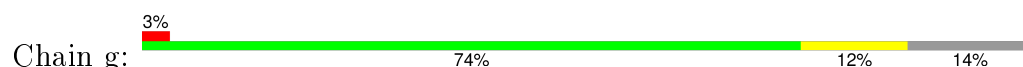




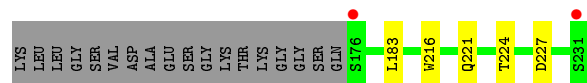
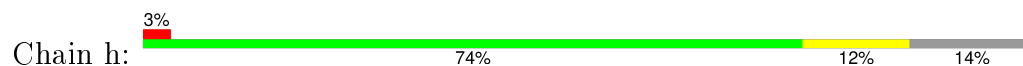
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



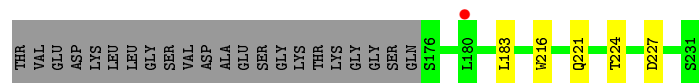
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



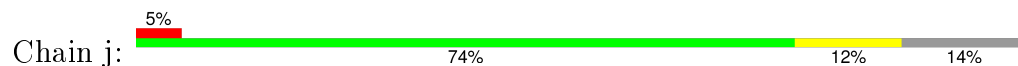
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

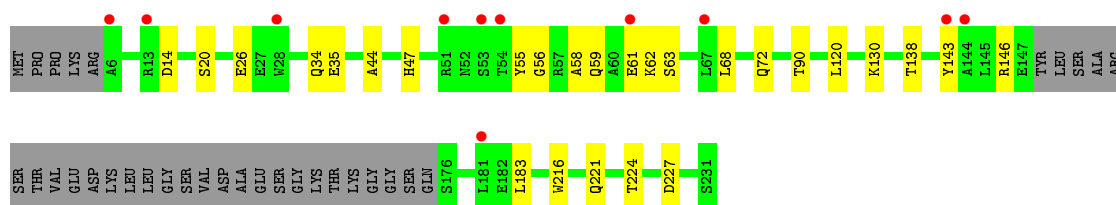


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

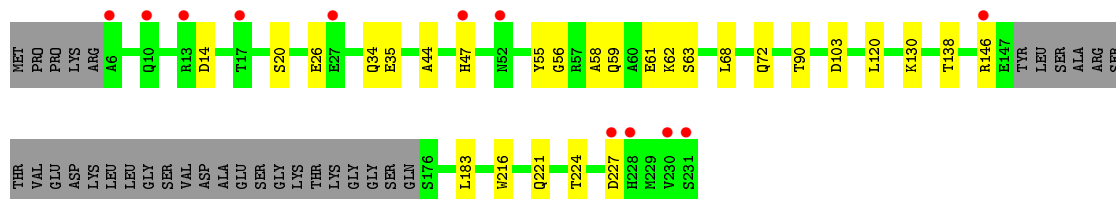
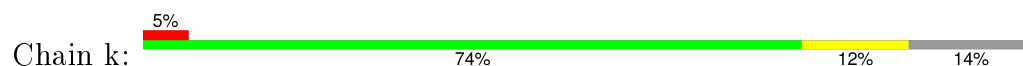


• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26

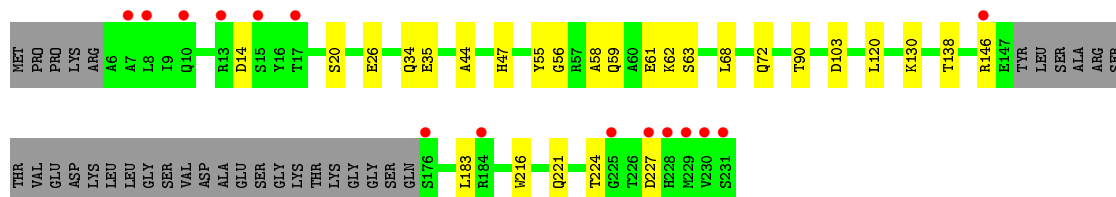




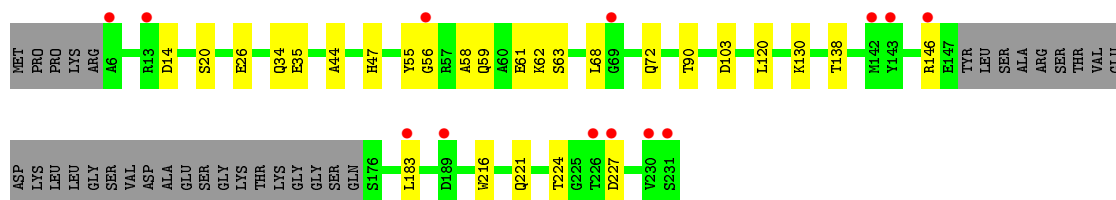
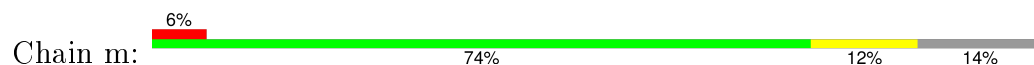
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



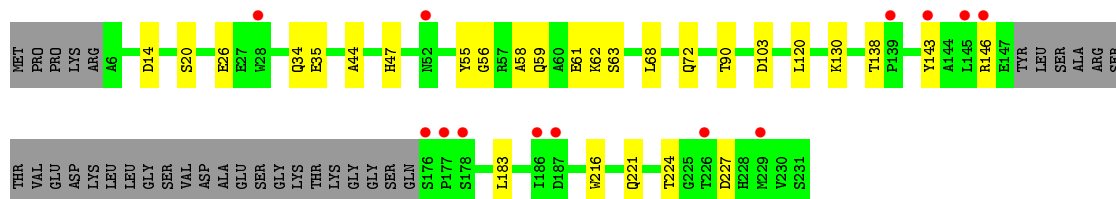
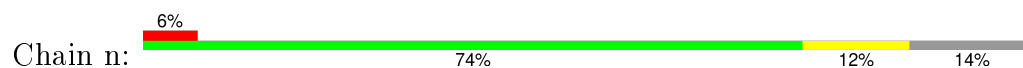
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



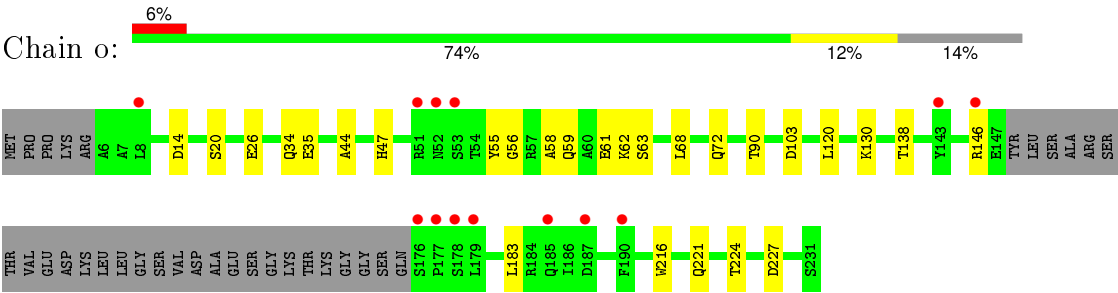
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



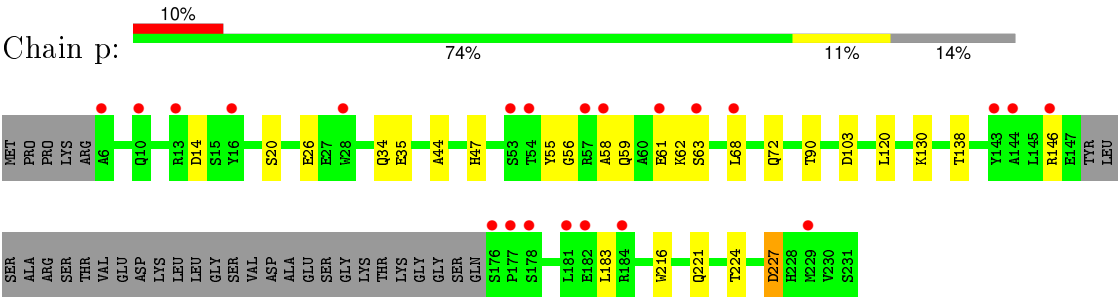
• Molecule 15: PROTEASOME ACTIVATOR PROTEIN PA26



• 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, α , β , γ	192.96 Å 232.13 Å 296.77 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.25 Å)	Xtriage
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%)	DCC
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 189495 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	70622	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Continued on next page...

Continued from previous page...

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

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	A	1881	0	1876	179	0
1	O	1881	0	1876	185	0
2	B	1868	0	1866	121	0
2	P	1868	0	1866	120	0
3	C	1868	0	1860	112	0
3	Q	1868	0	1860	110	0
4	D	1862	0	1866	88	0
4	R	1862	0	1866	82	0
5	E	1871	0	1840	91	0
5	S	1871	0	1840	85	0
6	F	1795	0	1797	107	0
6	T	1795	0	1797	101	0
7	G	1869	0	1864	138	0
7	U	1869	0	1864	139	0
8	H	1510	0	1476	121	0
8	V	1510	0	1476	115	0
9	I	1684	0	1688	84	0
9	W	1684	0	1688	104	0
10	J	1581	0	1574	65	0
10	X	1581	0	1574	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1585	0	1590	79	0
11	Y	1585	0	1590	73	0
12	L	1646	0	1595	52	0
12	Z	1646	0	1595	68	0
13	M	1757	0	1711	74	0
13	a	1757	0	1710	0	0
14	N	1824	0	1832	124	0
14	b	1824	0	1832	0	0
15	c	1529	0	1545	0	0
15	d	1529	0	1545	0	0
15	e	1529	0	1545	0	0
15	f	1529	0	1545	0	0
15	g	1529	0	1545	0	0
15	h	1529	0	1545	0	0
15	i	1529	0	1545	0	0
15	j	1529	0	1545	0	0
15	k	1529	0	1545	0	0
15	l	1529	0	1545	0	0
15	m	1529	0	1545	0	0
15	n	1529	0	1545	0	0
15	o	1529	0	1545	0	0
15	p	1529	0	1545	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	J	2	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	U	1	0	0	0	0
16	V	1	0	0	0	0
16	W	1	0	0	0	0
16	X	2	0	0	0	0
16	Z	1	0	0	0	0
16	a	1	0	0	0	0
All	All	70622	0	70499	2521	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 30.

The worst 5 of 2521 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)
2:B:46:ALA:HB2	2:B:211:LEU:HD12	1.34	1.10
2:P:46:ALA:HB2	2:P:211:LEU:HD12	1.37	1.05
8:H:13:ILE:HG12	8:H:177:VAL:HA	1.41	1.03
9:I:103:VAL:HG12	9:I:108:SER:HA	1.39	1.00
8:H:107:LYS:HD2	8:H:108:GLY:H	1.26	0.96

There are no symmetry-related clashes.

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%)	1	6
1	O	236/252 (94%)	174 (74%)	42 (18%)	20 (8%)	1	6
2	B	245/250 (98%)	170 (69%)	56 (23%)	19 (8%)	1	8
2	P	245/250 (98%)	174 (71%)	53 (22%)	18 (7%)	1	9
3	C	239/245 (98%)	191 (80%)	29 (12%)	19 (8%)	1	8
3	Q	239/245 (98%)	187 (78%)	32 (13%)	20 (8%)	1	6
4	D	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	2	13
4	R	237/254 (93%)	186 (78%)	36 (15%)	15 (6%)	2	13
5	E	242/260 (93%)	192 (79%)	36 (15%)	14 (6%)	2	17
5	S	242/260 (93%)	192 (79%)	35 (14%)	15 (6%)	2	14
6	F	231/234 (99%)	189 (82%)	36 (16%)	6 (3%)	7	40
6	T	231/234 (99%)	190 (82%)	32 (14%)	9 (4%)	4	28
7	G	238/287 (83%)	193 (81%)	37 (16%)	8 (3%)	5	31
7	U	238/287 (83%)	194 (82%)	34 (14%)	10 (4%)	3	26
8	H	194/196 (99%)	148 (76%)	30 (16%)	16 (8%)	1	7
8	V	194/196 (99%)	147 (76%)	34 (18%)	13 (7%)	1	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	220/232 (95%)	178 (81%)	27 (12%)	15 (7%)	1	11
9	W	220/232 (95%)	176 (80%)	31 (14%)	13 (6%)	2	16
10	J	202/205 (98%)	165 (82%)	33 (16%)	4 (2%)	9	48
10	X	202/205 (98%)	168 (83%)	30 (15%)	4 (2%)	9	48
11	K	196/198 (99%)	163 (83%)	24 (12%)	9 (5%)	3	23
11	Y	196/198 (99%)	160 (82%)	28 (14%)	8 (4%)	3	27
12	L	210/212 (99%)	180 (86%)	27 (13%)	3 (1%)	14	57
12	Z	210/212 (99%)	178 (85%)	29 (14%)	3 (1%)	14	57
13	M	220/222 (99%)	188 (86%)	24 (11%)	8 (4%)	4	30
13	a	220/222 (99%)	186 (84%)	25 (11%)	9 (4%)	3	27
14	N	231/233 (99%)	169 (73%)	43 (19%)	19 (8%)	1	7
14	b	231/233 (99%)	170 (74%)	40 (17%)	21 (9%)	1	5
15	c	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	19
15	d	194/231 (84%)	162 (84%)	21 (11%)	11 (6%)	2	17
15	e	194/231 (84%)	161 (83%)	22 (11%)	11 (6%)	2	17
15	f	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	19
15	g	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	19
15	h	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	19
15	i	194/231 (84%)	162 (84%)	22 (11%)	10 (5%)	2	19
15	j	194/231 (84%)	162 (84%)	23 (12%)	9 (5%)	3	23
15	k	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	2	19
15	l	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	2	19
15	m	194/231 (84%)	160 (82%)	24 (12%)	10 (5%)	2	19
15	n	194/231 (84%)	161 (83%)	23 (12%)	10 (5%)	2	19
15	o	194/231 (84%)	159 (82%)	25 (13%)	10 (5%)	2	19
15	p	194/231 (84%)	163 (84%)	20 (10%)	11 (6%)	2	17
All	All	8998/9794 (92%)	7221 (80%)	1282 (14%)	495 (6%)	2	18

5 of 495 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	19	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	60	PRO
1	A	115	ASP
1	A	221	ASN

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	A	204/210 (97%)	173 (85%)	31 (15%)	3	17
1	O	204/210 (97%)	174 (85%)	30 (15%)	4	18
2	B	200/209 (96%)	169 (84%)	31 (16%)	3	15
2	P	200/209 (96%)	167 (84%)	33 (16%)	3	13
3	C	198/204 (97%)	168 (85%)	30 (15%)	3	17
3	Q	198/204 (97%)	169 (85%)	29 (15%)	4	19
4	D	209/226 (92%)	175 (84%)	34 (16%)	3	14
4	R	209/226 (92%)	176 (84%)	33 (16%)	3	15
5	E	198/215 (92%)	170 (86%)	28 (14%)	4	20
5	S	198/215 (92%)	170 (86%)	28 (14%)	4	20
6	F	192/193 (100%)	164 (85%)	28 (15%)	4	19
6	T	192/193 (100%)	164 (85%)	28 (15%)	4	19
7	G	199/238 (84%)	167 (84%)	32 (16%)	3	14
7	U	199/238 (84%)	165 (83%)	34 (17%)	2	12
8	H	161/162 (99%)	132 (82%)	29 (18%)	2	11
8	V	161/162 (99%)	133 (83%)	28 (17%)	2	12
9	I	181/190 (95%)	156 (86%)	25 (14%)	4	21
9	W	181/190 (95%)	157 (87%)	24 (13%)	5	23
10	J	172/173 (99%)	149 (87%)	23 (13%)	5	22
10	X	172/173 (99%)	150 (87%)	22 (13%)	5	25
11	K	175/175 (100%)	155 (89%)	20 (11%)	7	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	175/175 (100%)	154 (88%)	21 (12%)	6	28
12	L	169/169 (100%)	147 (87%)	22 (13%)	5	24
12	Z	169/169 (100%)	148 (88%)	21 (12%)	6	27
13	M	185/185 (100%)	163 (88%)	22 (12%)	6	28
13	a	185/185 (100%)	162 (88%)	23 (12%)	6	27
14	N	199/199 (100%)	169 (85%)	30 (15%)	3	17
14	b	199/199 (100%)	167 (84%)	32 (16%)	3	14
15	c	163/190 (86%)	146 (90%)	17 (10%)	9	35
15	d	163/190 (86%)	146 (90%)	17 (10%)	9	35
15	e	163/190 (86%)	146 (90%)	17 (10%)	9	35
15	f	163/190 (86%)	147 (90%)	16 (10%)	10	38
15	g	163/190 (86%)	147 (90%)	16 (10%)	10	38
15	h	163/190 (86%)	147 (90%)	16 (10%)	10	38
15	i	163/190 (86%)	146 (90%)	17 (10%)	9	35
15	j	163/190 (86%)	146 (90%)	17 (10%)	9	35
15	k	163/190 (86%)	147 (90%)	16 (10%)	10	38
15	l	163/190 (86%)	147 (90%)	16 (10%)	10	38
15	m	163/190 (86%)	147 (90%)	16 (10%)	10	38
15	n	163/190 (86%)	146 (90%)	17 (10%)	9	35
15	o	163/190 (86%)	147 (90%)	16 (10%)	10	38
15	p	163/190 (86%)	147 (90%)	16 (10%)	10	38
All	All	7566/8156 (93%)	6565 (87%)	1001 (13%)	5	23

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

Mol	Chain	Res	Type
3	Q	50	ARG
6	T	198	SER
15	l	55	TYR
3	Q	175	LEU
4	R	242	GLU

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

Mol	Chain	Res	Type
5	S	23	GLN
9	W	144	GLN
15	m	80	ASN
6	T	4	ASN
7	U	143	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 carbohydrates 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 ⓘ

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	A	238/252 (94%)	0.14	8 (3%) 49 34	45, 88, 99, 100	0
1	O	238/252 (94%)	0.14	7 (2%) 55 41	51, 89, 99, 100	0
2	B	247/250 (98%)	0.07	4 (1%) 74 62	39, 78, 96, 100	0
2	P	247/250 (98%)	-0.05	3 (1%) 81 69	46, 81, 98, 100	0
3	C	241/245 (98%)	-0.07	4 (1%) 73 60	35, 71, 99, 100	0
3	Q	241/245 (98%)	0.03	9 (3%) 45 30	37, 77, 99, 100	0
4	D	239/254 (94%)	-0.06	5 (2%) 67 52	34, 69, 98, 100	0
4	R	239/254 (94%)	-0.06	5 (2%) 67 52	37, 74, 99, 100	0
5	E	244/260 (93%)	-0.02	12 (4%) 33 20	29, 67, 98, 100	0
5	S	244/260 (93%)	0.04	9 (3%) 45 30	41, 72, 99, 100	0
6	F	233/234 (99%)	-0.23	0 100 100	33, 69, 87, 98	0
6	T	233/234 (99%)	-0.03	2 (0%) 85 78	45, 74, 92, 100	0
7	G	240/287 (83%)	0.11	6 (2%) 61 47	45, 82, 98, 100	0
7	U	240/287 (83%)	0.20	6 (2%) 61 47	52, 85, 99, 100	0
8	H	196/196 (100%)	-0.04	3 (1%) 76 63	51, 79, 97, 100	0
8	V	196/196 (100%)	0.05	5 (2%) 59 45	56, 81, 98, 100	0
9	I	222/232 (95%)	-0.14	4 (1%) 71 58	44, 74, 95, 100	0
9	W	222/232 (95%)	-0.08	5 (2%) 64 49	44, 75, 93, 100	0
10	J	204/205 (99%)	-0.35	3 (1%) 76 63	29, 60, 85, 100	0
10	X	204/205 (99%)	-0.40	1 (0%) 91 87	33, 60, 82, 95	0
11	K	198/198 (100%)	-0.25	5 (2%) 61 47	23, 52, 80, 100	0
11	Y	198/198 (100%)	-0.33	2 (1%) 84 75	30, 56, 84, 100	0
12	L	212/212 (100%)	-0.40	2 (0%) 85 78	30, 52, 72, 96	0
12	Z	212/212 (100%)	-0.52	0 100 100	31, 52, 76, 92	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	222/222 (100%)	-0.33	1 (0%) 91 87	28, 60, 79, 97	0
13	a	222/222 (100%)	-0.29	2 (0%) 85 78	30, 61, 85, 99	0
14	N	233/233 (100%)	-0.13	3 (1%) 79 67	37, 72, 95, 99	0
14	b	233/233 (100%)	-0.06	2 (0%) 85 78	39, 74, 96, 100	0
15	c	198/231 (85%)	0.28	5 (2%) 61 47	58, 90, 99, 100	0
15	d	198/231 (85%)	0.47	19 (9%) 10 6	65, 92, 100, 100	0
15	e	198/231 (85%)	0.43	19 (9%) 10 6	58, 91, 100, 100	0
15	f	198/231 (85%)	0.18	7 (3%) 48 32	47, 89, 99, 100	0
15	g	198/231 (85%)	0.17	7 (3%) 48 32	48, 88, 99, 100	0
15	h	198/231 (85%)	0.29	8 (4%) 42 27	57, 86, 99, 100	0
15	i	198/231 (85%)	0.28	7 (3%) 48 32	56, 91, 100, 100	0
15	j	198/231 (85%)	0.41	11 (5%) 28 16	60, 94, 100, 100	0
15	k	198/231 (85%)	0.38	12 (6%) 25 13	65, 94, 100, 100	0
15	l	198/231 (85%)	0.32	15 (7%) 17 9	56, 93, 100, 100	0
15	m	198/231 (85%)	0.30	13 (6%) 22 12	56, 94, 100, 100	0
15	n	198/231 (85%)	0.34	13 (6%) 22 12	64, 94, 100, 100	0
15	o	198/231 (85%)	0.43	13 (6%) 22 12	70, 93, 100, 100	0
15	p	198/231 (85%)	0.52	22 (11%) 7 4	67, 95, 100, 100	0
All	All	9110/9794 (93%)	0.03	289 (3%) 51 36	23, 79, 99, 100	0

The worst 5 of 289 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	S	129	GLY	6.7
3	Q	245	THR	6.3
15	k	231	SER	5.9
5	E	128	SER	5.5
5	S	126	GLY	5.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
16	MG	H	1002	1/1	0.72	0.38	6.05	81,81,81,81	0
16	MG	J	1005	1/1	0.97	0.26	5.42	37,37,37,37	0
16	MG	X	1012	1/1	0.82	0.29	2.61	56,56,56,56	0
16	MG	L	1003	1/1	0.89	0.23	1.67	43,43,43,43	0
16	MG	U	1014	1/1	0.77	0.30	0.73	65,65,65,65	0
16	MG	V	1009	1/1	0.89	0.18	-0.62	39,39,39,39	0
16	MG	a	1011	1/1	0.97	0.06	-1.76	49,49,49,49	0
16	MG	M	1004	1/1	0.98	0.07	-2.17	26,26,26,26	0
16	MG	G	1007	1/1	0.91	0.10	-2.81	38,38,38,38	0
16	MG	I	1001	1/1	0.88	0.16	-3.61	67,67,67,67	0
16	MG	Z	1010	1/1	0.98	0.08	-3.80	38,38,38,38	0
16	MG	W	1008	1/1	0.95	0.08	-5.08	67,67,67,67	0
16	MG	J	1006	1/1	0.92	0.09	-	24,24,24,24	0
16	MG	X	1013	1/1	0.87	0.23	-	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.