wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:43 AM GMT

PDB ID	:	3MKA
Title	:	Crystal Structure of Mycobacterium Tuberculosis Proteasome with propetide and an T1A mutation at beta-subunit
Authors	:	Li, D.; Li, H.
Deposited on	:	2010-04-14
Resolution	:	2.51 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

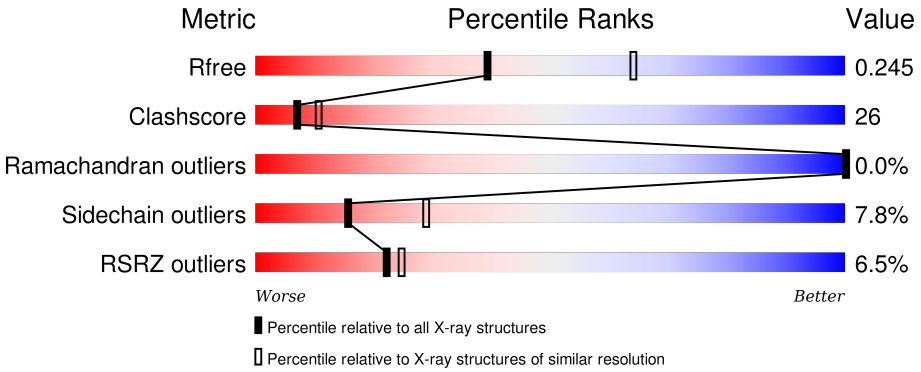
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	248	13% 54% 29% • 12%
1	A	248	5% 49% 38% • 10%
1	B	248	7% 53% 31% 5% 11%
1	D	248	8% 54% 31% 5% 10%
1	F	248	10% 54% 31% • 11%

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Mol	Chain	Length	Quality of chain
1	I	248	6% 55% 27% 5% 13%
1	K	248	16% 48% 36% 6% 11%
1	M	248	5% 56% 29% 5% 10%
1	O	248	10% 51% 33% • 12%
1	Q	248	8% 48% 36% 6% 10%
1	S	248	8% 50% 35% • 12%
1	U	248	7% 50% 33% 6% 11%
1	W	248	8% 54% 29% 5% 11%
1	Y	248	8% 53% 33% 5% 10%
2	2	291	3% 61% 21% • 15%
2	C	291	4% 59% 24% • 14%
2	E	291	5% 54% 28% • 15%
2	G	291	2% 64% 21% • 14%
2	H	291	5% 60% 24% • 14%
2	J	291	4% 62% 22% • 13%
2	L	291	3% 57% 25% • 14%
2	N	291	3% 64% 20% • 13%
2	P	291	3% 61% 21% • 14%
2	R	291	3% 60% 23% • 15%
2	T	291	2% 62% 23% • 14%
2	V	291	% 63% 21% • 14%
2	X	291	4% 59% 23% • 14%
2	Z	291	3% 57% 25% • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49801 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1713	1078	310	322	3			
1	B	220	Total	C	N	O	S	0	0	0
			1695	1064	308	320	3			
1	D	222	Total	C	N	O	S	0	0	0
			1717	1082	310	322	3			
1	F	221	Total	C	N	O	S	0	0	0
			1706	1073	309	321	3			
1	I	217	Total	C	N	O	S	0	0	0
			1680	1055	305	317	3			
1	K	221	Total	C	N	O	S	0	0	0
			1705	1072	309	321	3			
1	M	224	Total	C	N	O	S	0	0	0
			1730	1090	312	325	3			
1	O	218	Total	C	N	O	S	0	0	0
			1675	1049	306	317	3			
1	Q	222	Total	C	N	O	S	0	0	0
			1716	1081	310	322	3			
1	S	219	Total	C	N	O	S	0	0	0
			1686	1058	307	318	3			
1	U	221	Total	C	N	O	S	0	0	0
			1706	1073	309	321	3			
1	W	221	Total	C	N	O	S	0	0	0
			1710	1078	309	320	3			
1	Y	224	Total	C	N	O	S	0	0	0
			1730	1090	312	325	3			
1	1	219	Total	C	N	O	S	0	0	0
			1693	1065	307	318	3			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	250	Total	C	N	O	S	0	0	0
			1853	1165	320	363	5			
2	E	248	Total	C	N	O	S	0	0	0
			1834	1153	317	359	5			
2	G	251	Total	C	N	O	S	0	0	0
			1858	1168	321	364	5			
2	H	249	Total	C	N	O	S	0	0	0
			1844	1159	319	361	5			
2	J	252	Total	C	N	O	S	0	0	0
			1863	1170	322	366	5			
2	L	251	Total	C	N	O	S	0	0	0
			1857	1167	321	364	5			
2	N	252	Total	C	N	O	S	0	0	0
			1863	1170	322	366	5			
2	P	250	Total	C	N	O	S	0	0	0
			1853	1165	320	363	5			
2	R	246	Total	C	N	O	S	0	0	0
			1822	1145	315	357	5			
2	T	250	Total	C	N	O	S	0	0	0
			1854	1165	320	364	5			
2	V	249	Total	C	N	O	S	0	0	0
			1843	1158	319	361	5			
2	X	249	Total	C	N	O	S	0	0	0
			1848	1162	319	362	5			
2	Z	245	Total	C	N	O	S	0	0	0
			1817	1142	314	356	5			
2	2	246	Total	C	N	O	S	0	0	0
			1829	1150	316	358	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	301	ALA	THR	ENGINEERED	UNP O33245
E	301	ALA	THR	ENGINEERED	UNP O33245
G	301	ALA	THR	ENGINEERED	UNP O33245
H	301	ALA	THR	ENGINEERED	UNP O33245
J	301	ALA	THR	ENGINEERED	UNP O33245
L	301	ALA	THR	ENGINEERED	UNP O33245
N	301	ALA	THR	ENGINEERED	UNP O33245
P	301	ALA	THR	ENGINEERED	UNP O33245
R	301	ALA	THR	ENGINEERED	UNP O33245
T	301	ALA	THR	ENGINEERED	UNP O33245
V	301	ALA	THR	ENGINEERED	UNP O33245
X	301	ALA	THR	ENGINEERED	UNP O33245

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	301	ALA	THR	ENGINEERED	UNP O33245
2	301	ALA	THR	ENGINEERED	UNP O33245

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	2	Total O 2 2	0	0
3	C	3	Total O 3 3	0	0
3	D	3	Total O 3 3	0	0
3	E	1	Total O 1 1	0	0
3	F	4	Total O 4 4	0	0
3	G	13	Total O 13 13	0	0
3	H	3	Total O 3 3	0	0
3	I	2	Total O 2 2	0	0
3	J	3	Total O 3 3	0	0
3	K	4	Total O 4 4	0	0
3	L	2	Total O 2 2	0	0
3	M	5	Total O 5 5	0	0
3	N	4	Total O 4 4	0	0
3	O	1	Total O 1 1	0	0
3	P	5	Total O 5 5	0	0
3	R	1	Total O 1 1	0	0
3	S	3	Total O 3 3	0	0

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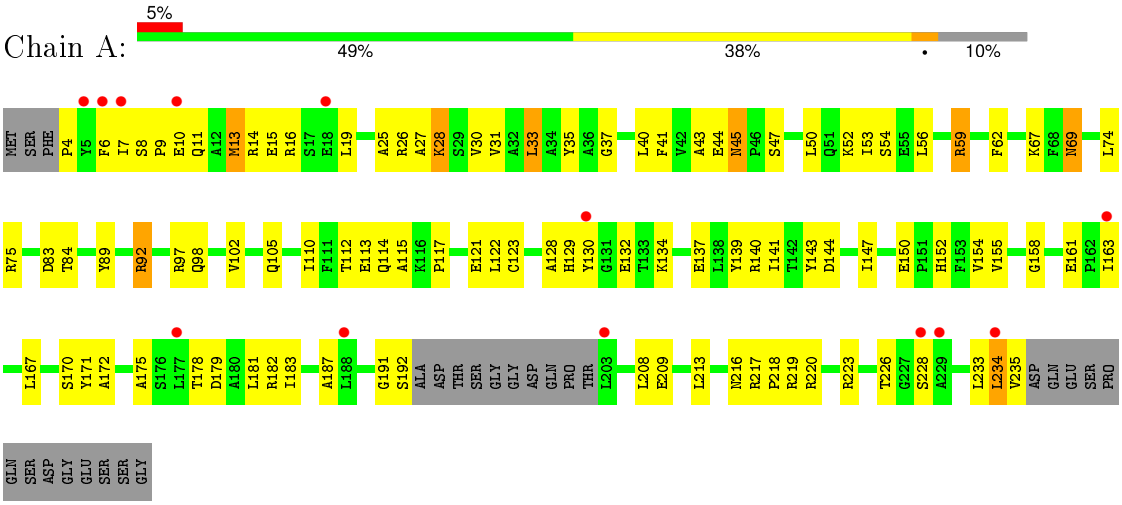
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	T	3	Total O 3 3	0	0
3	U	2	Total O 2 2	0	0
3	V	4	Total O 4 4	0	0
3	W	6	Total O 6 6	0	0
3	X	2	Total O 2 2	0	0
3	Y	6	Total O 6 6	0	0
3	Z	5	Total O 5 5	0	0
3	2	5	Total O 5 5	0	0
3	1	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

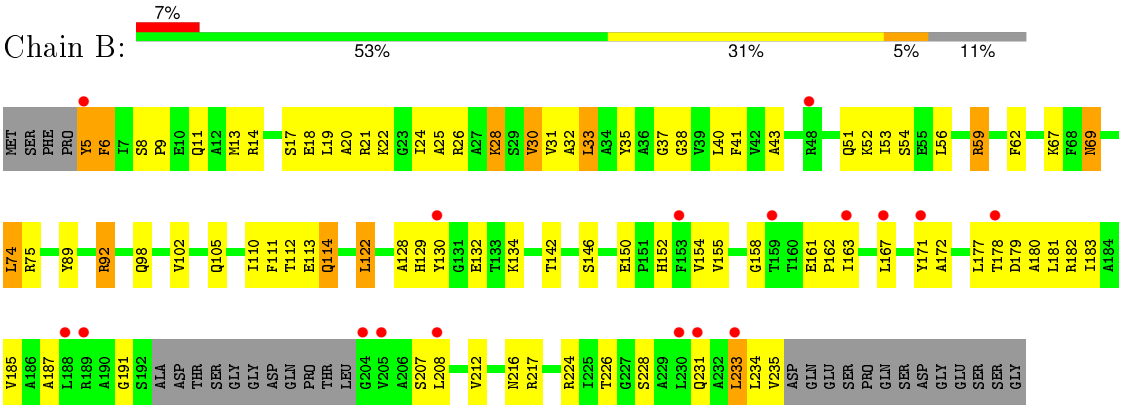
- Molecule 1: Proteasome subunit alpha

Chain A:



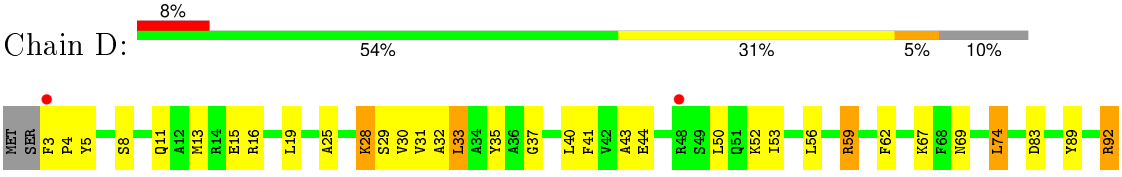
- Molecule 1: Proteasome subunit alpha

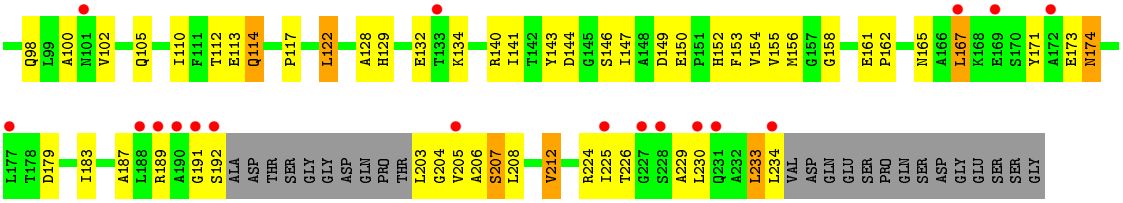
Chain B:



- Molecule 1: Proteasome subunit alpha

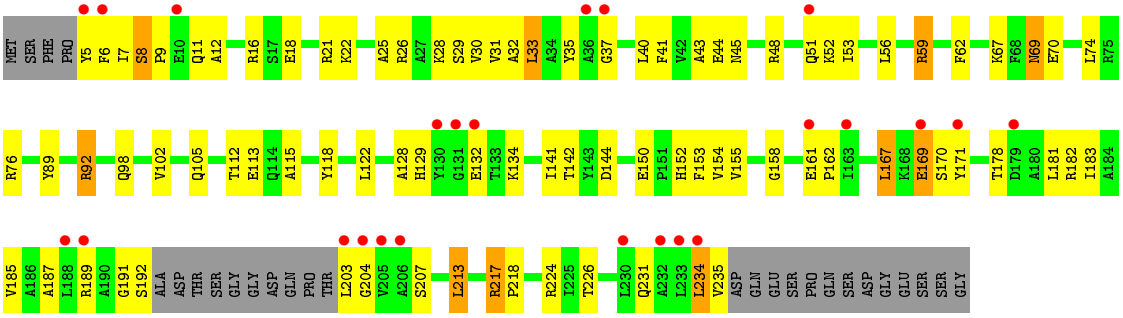
Chain D:





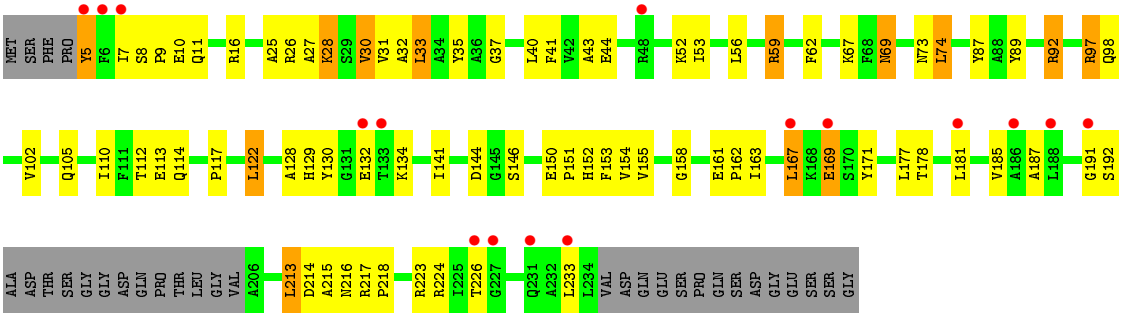
• Molecule 1: Proteasome subunit alpha

Chain F:



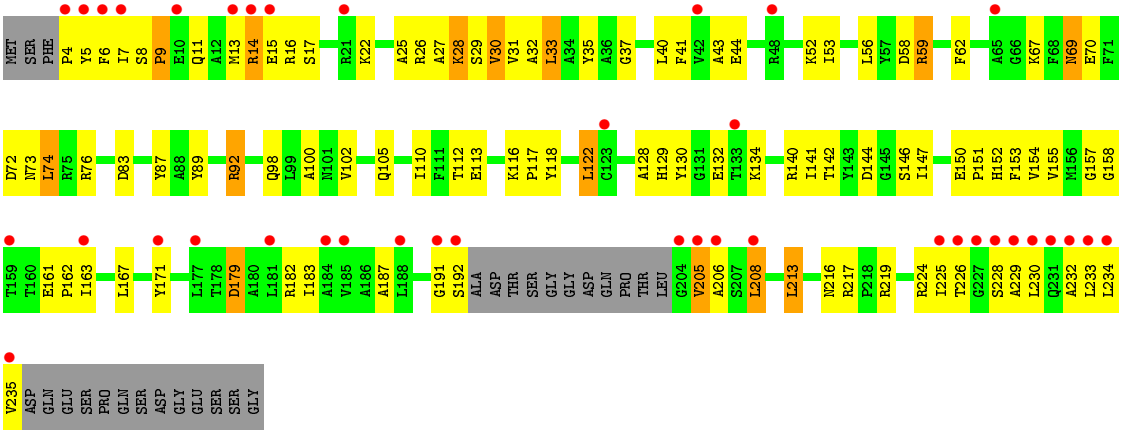
• Molecule 1: Proteasome subunit alpha

Chain I:



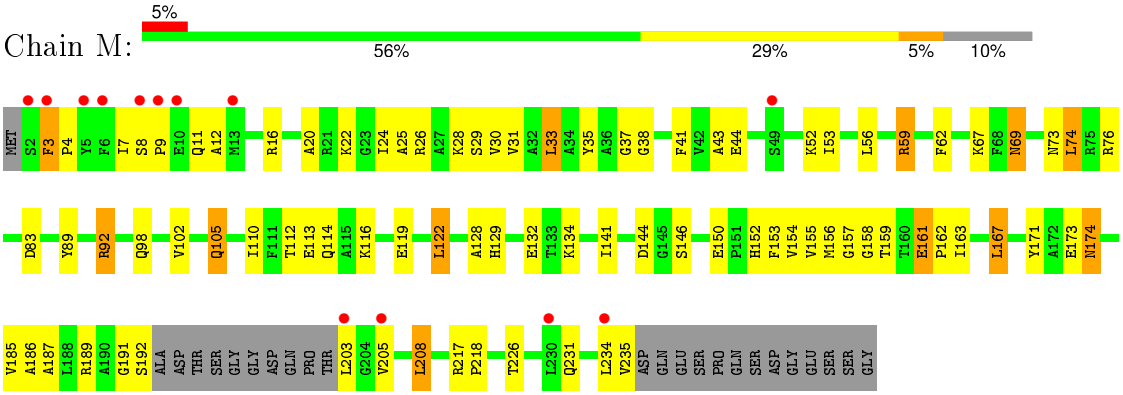
• Molecule 1: Proteasome subunit alpha

Chain K:



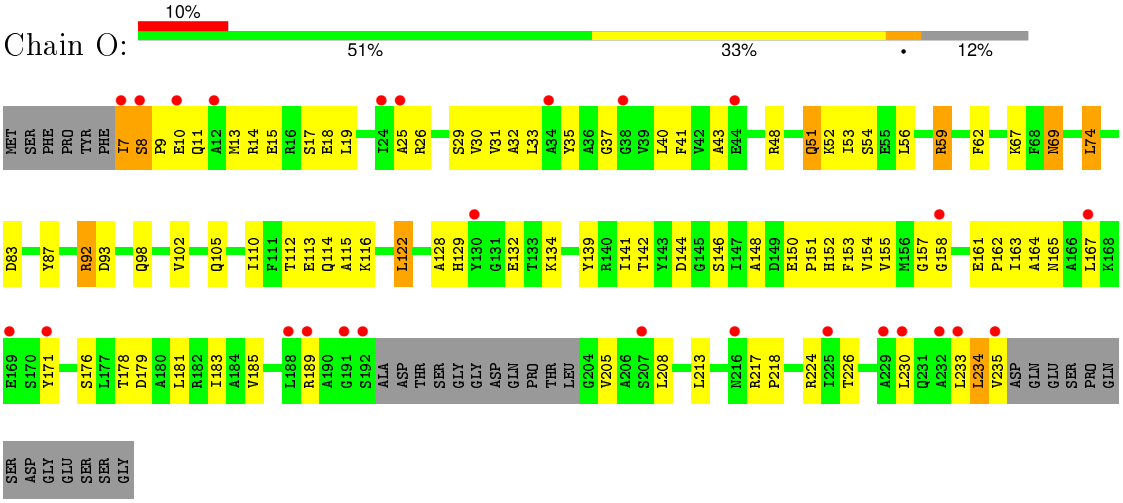
- Molecule 1: Proteasome subunit alpha

Chain M:



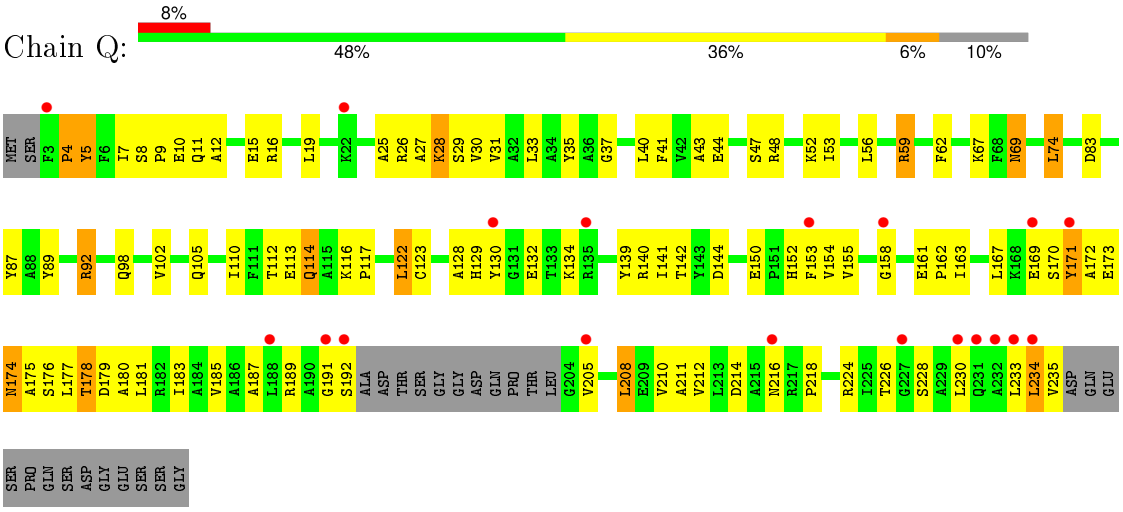
- Molecule 1: Proteasome subunit alpha

Chain O:



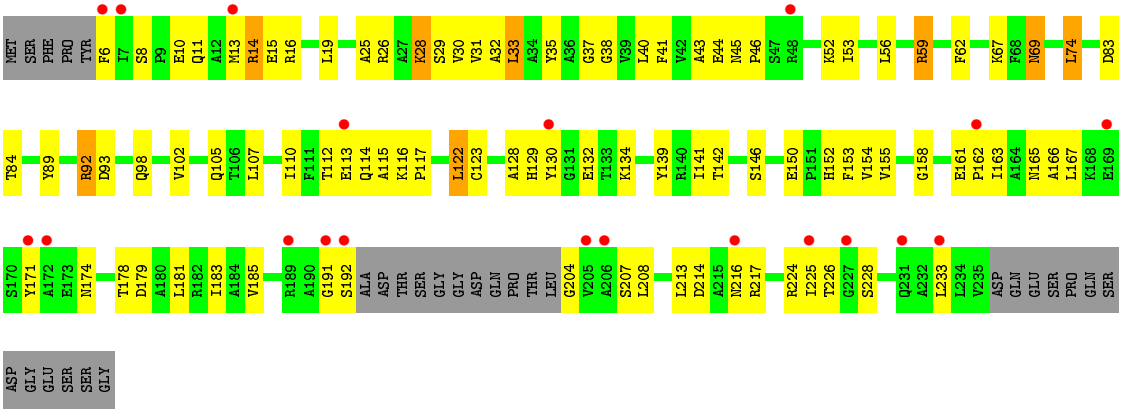
- Molecule 1: Proteasome subunit alpha

Chain Q:



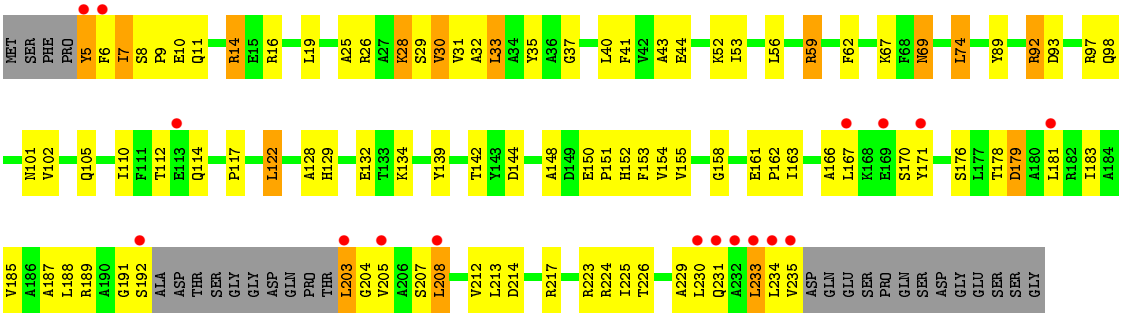
- Molecule 1: Proteasome subunit alpha

Chain S:



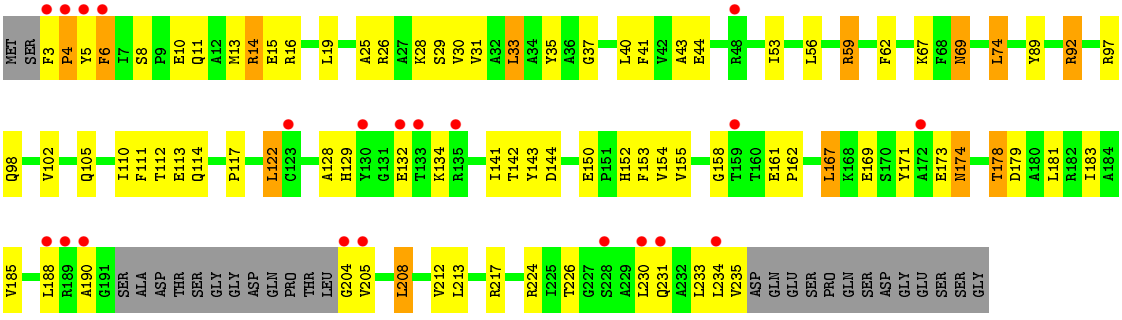
- Molecule 1: Proteasome subunit alpha

Chain U:



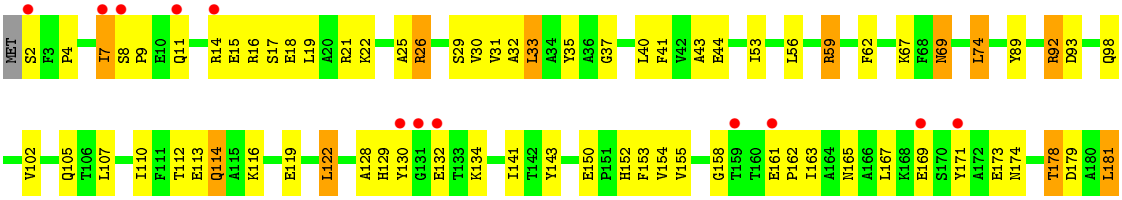
- Molecule 1: Proteasome subunit alpha

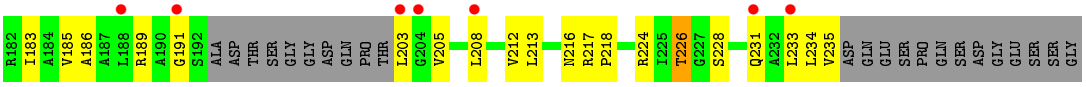
Chain W:



- Molecule 1: Proteasome subunit alpha

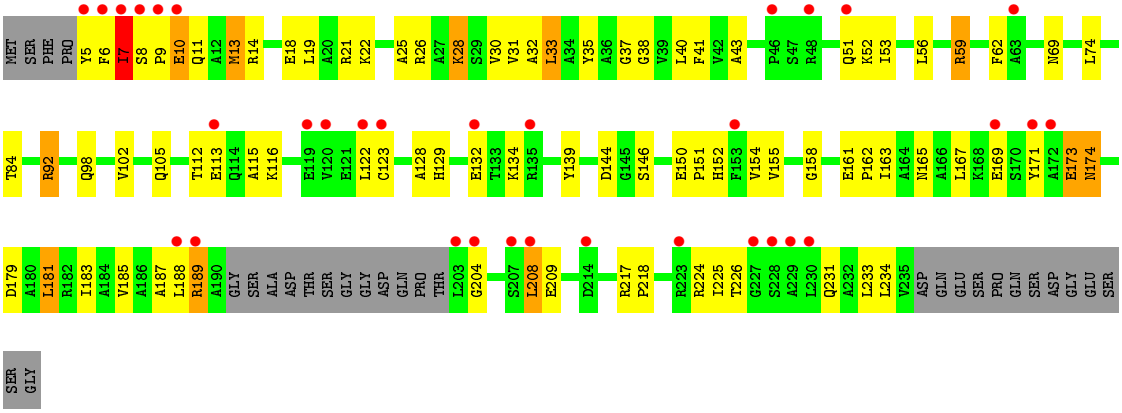
Chain Y:





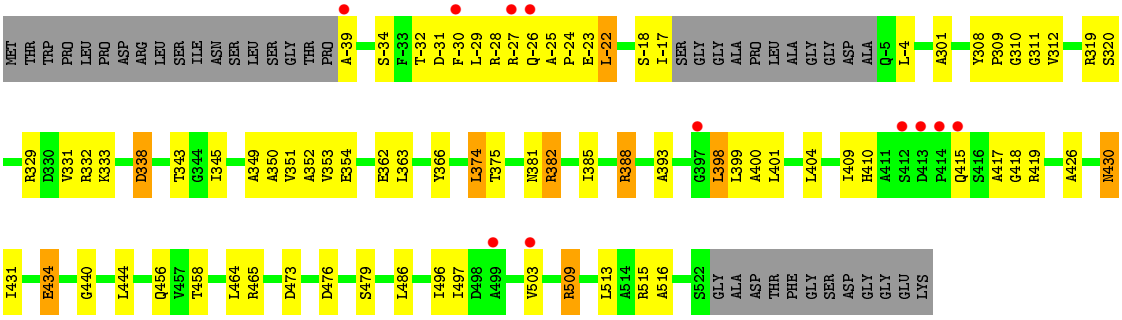
- Molecule 1: Proteasome subunit alpha

Chain 1:



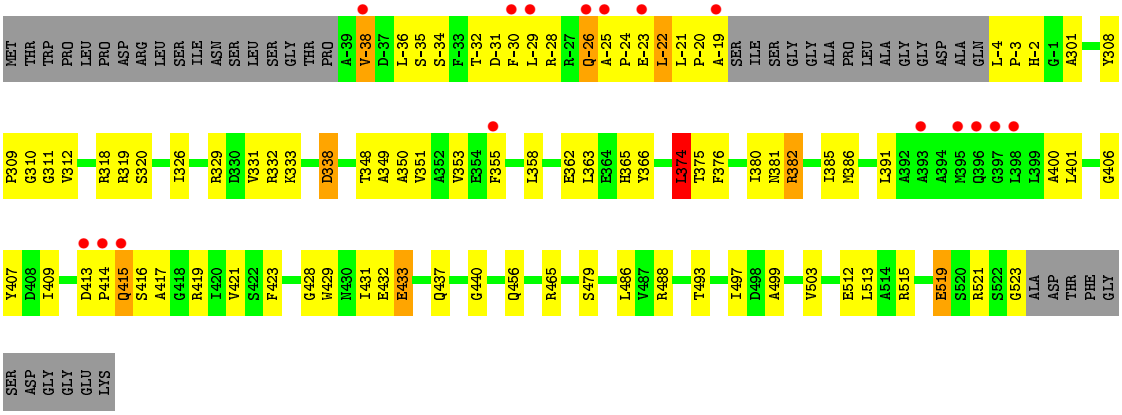
- Molecule 2: Proteasome subunit beta

Chain C:



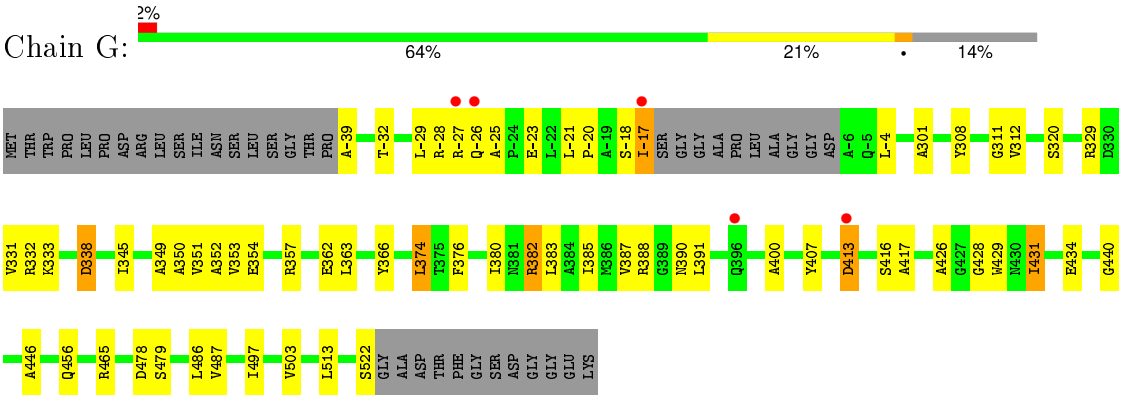
- Molecule 2: Proteasome subunit beta

Chain E:



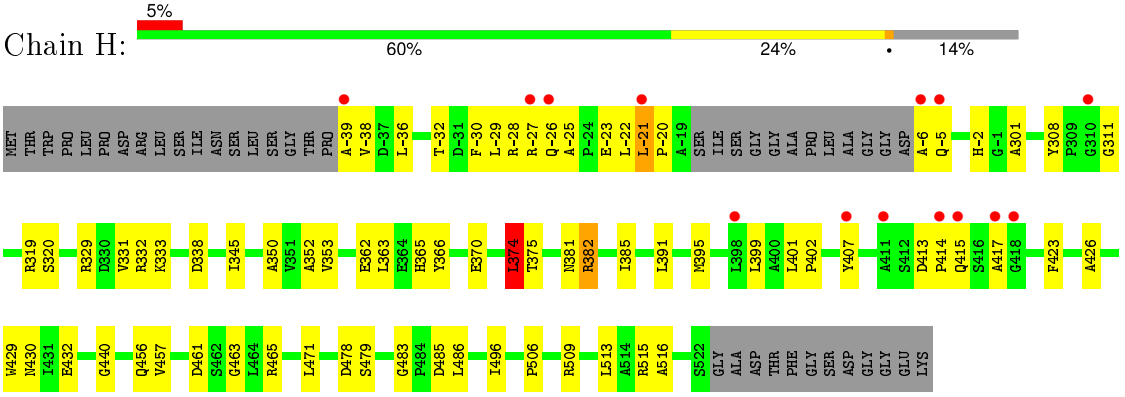
- Molecule 2: Proteasome subunit beta

Chain G:



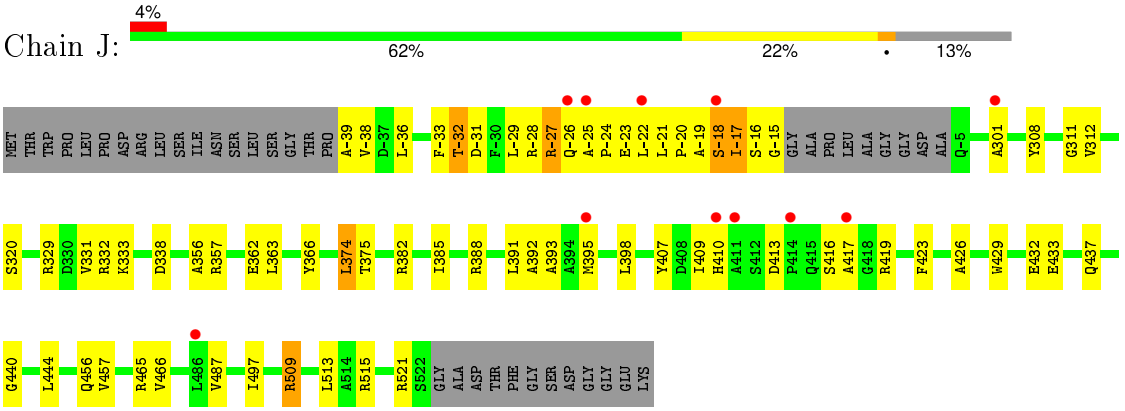
- Molecule 2: Proteasome subunit beta

Chain H:



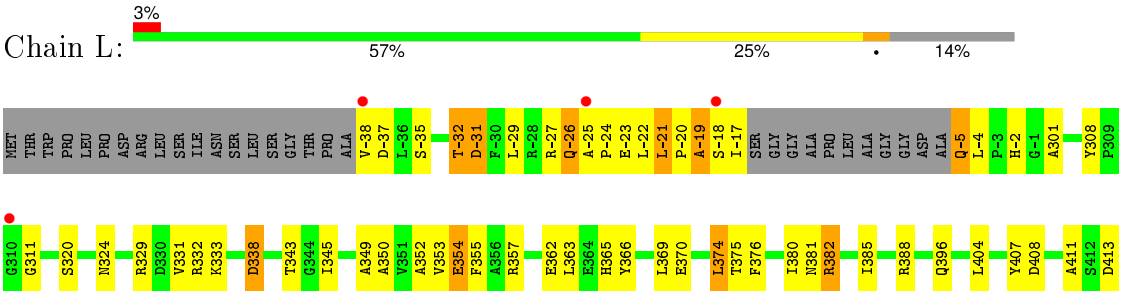
- Molecule 2: Proteasome subunit beta

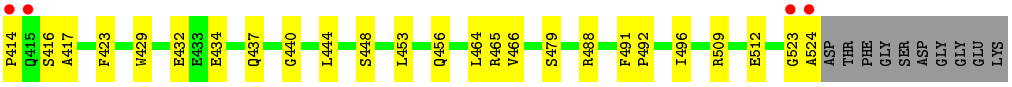
Chain J:



- Molecule 2: Proteasome subunit beta

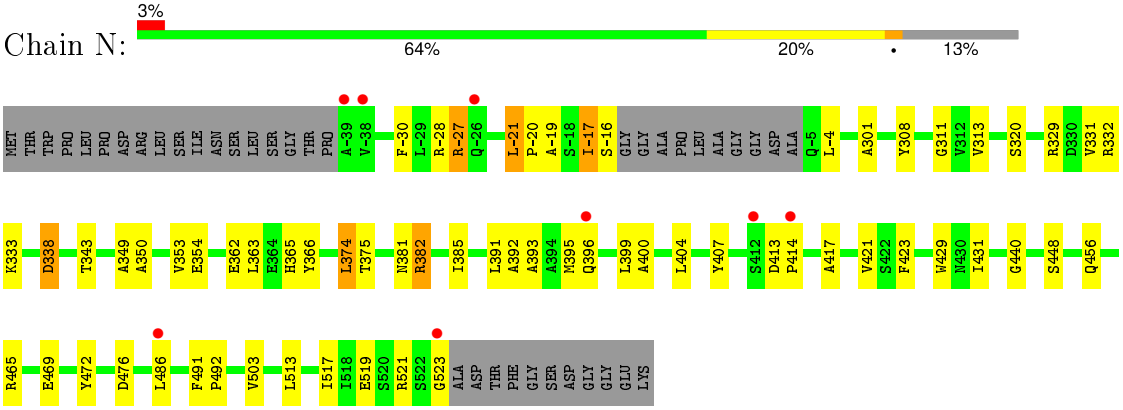
Chain L:





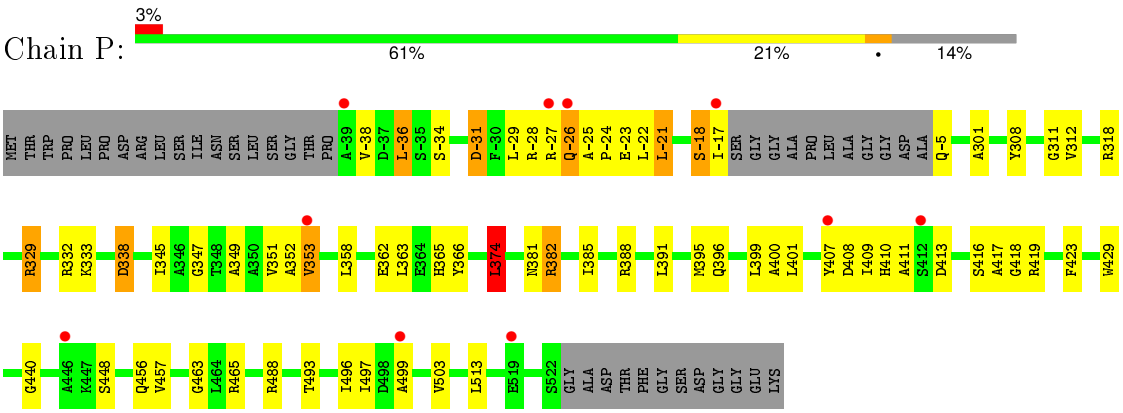
- Molecule 2: Proteasome subunit beta

Chain N:



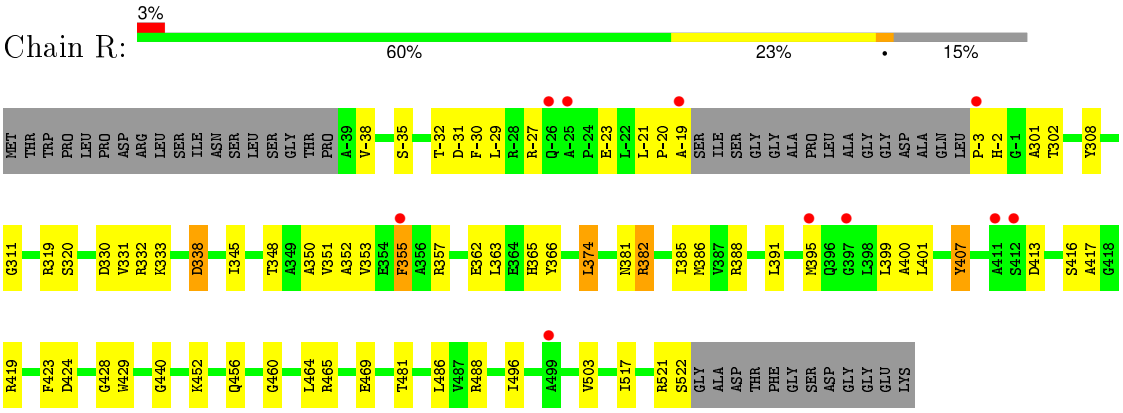
- Molecule 2: Proteasome subunit beta

Chain P:



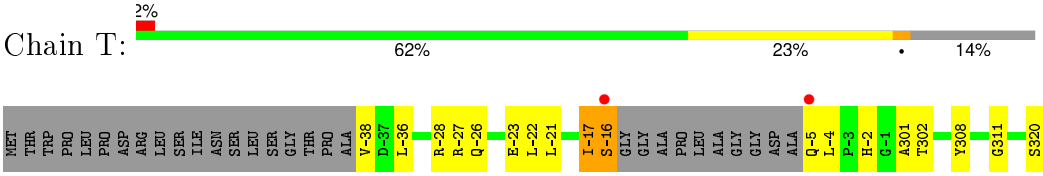
- Molecule 2: Proteasome subunit beta

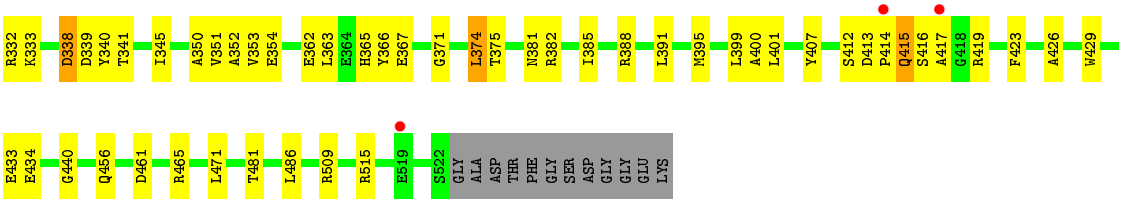
Chain R:



- Molecule 2: Proteasome subunit beta

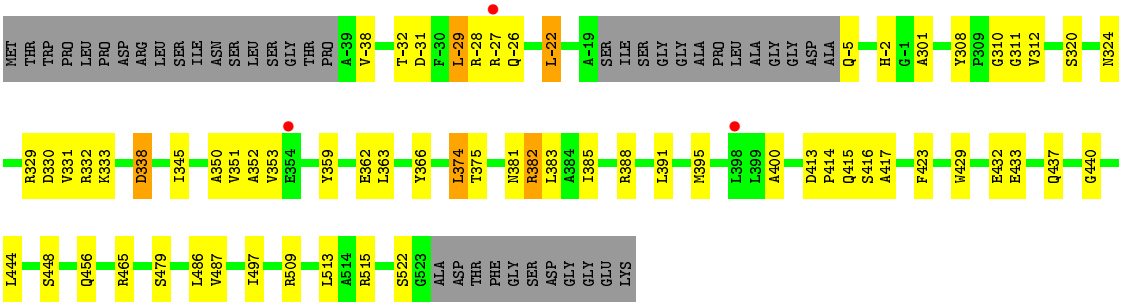
Chain T:





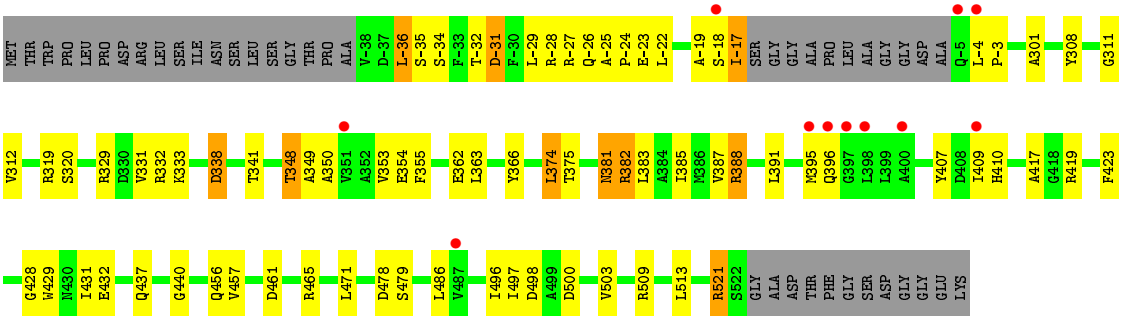
• Molecule 2: Proteasome subunit beta

Chain V:



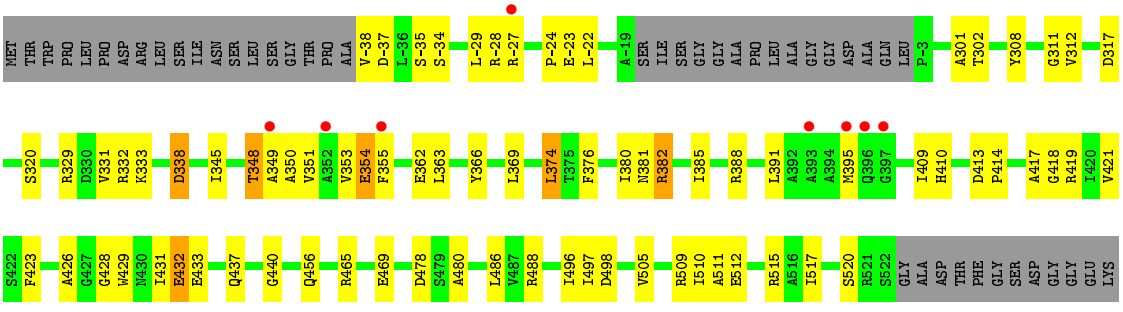
• Molecule 2: Proteasome subunit beta

Chain X:



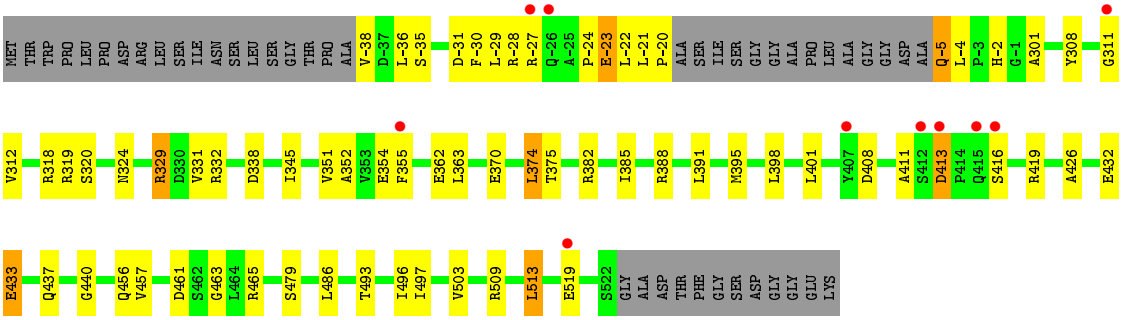
• Molecule 2: Proteasome subunit beta

Chain Z:



• Molecule 2: Proteasome subunit beta

Chain 2:


MET THR TRP PRO LEU PRO ASP ARG LEU SER ILE ASN SER LEU SER GLY THR PRO ALA V-38 D-37 L-36 S-35 D-31 F-30 L-29 R-28 R-27 Q-26 A-25 P-24 E-23 L-22 L-21 P-20 ALA SER ILE SER GLY GLY ALA PRO LEU ALA GLY GLY ASP ALA Q-5 L-4 P-3 H-2 G-1 A301 Y308 G311
V312 R318 R319 S320 N324 R329 D330 V331 R332 D338 I345 V351 A362 V353 E354 F355 E362 L363 E370 L374 T375 R382 I385 R388 L391 M395 L398 L401 Y407 D408 A411 S412 D413 P414 Q415 S416 R419 A426 E432
E433 Q437 G440 Q456 V457 D461 S462 G463 L464 R465 S479 L486 T493 I496 I497 V503 R509 L513 E519 S522 GLY ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	173.93Å 115.42Å 199.58Å 90.00° 112.89° 90.00°	Depositor
Resolution (Å)	29.77 – 2.51 35.04 – 2.51	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.77-2.51) 94.0 (35.04-2.51)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.247 0.215 , 0.245	Depositor DCC
R_{free} test set	11793 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.3	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 233933 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49801	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.72	0/1720	0.83	0/2325
1	A	0.72	0/1741	0.82	2/2353 (0.1%)
1	B	0.65	0/1722	0.77	0/2327
1	D	0.69	0/1746	0.86	1/2360 (0.0%)
1	F	0.73	0/1733	0.84	2/2342 (0.1%)
1	I	0.72	0/1707	0.86	2/2306 (0.1%)
1	K	0.67	0/1733	0.84	1/2342 (0.0%)
1	M	0.75	0/1759	0.83	1/2378 (0.0%)
1	O	0.66	0/1700	0.84	1/2297 (0.0%)
1	Q	0.69	0/1745	0.81	0/2359
1	S	0.68	0/1712	0.82	1/2313 (0.0%)
1	U	0.71	0/1733	0.84	1/2342 (0.0%)
1	W	0.74	0/1739	0.83	1/2351 (0.0%)
1	Y	0.69	0/1759	0.82	2/2378 (0.1%)
2	2	0.79	0/1858	0.87	0/2520
2	C	0.84	0/1882	0.84	1/2553 (0.0%)
2	E	0.74	0/1863	0.84	2/2527 (0.1%)
2	G	0.86	1/1887 (0.1%)	0.86	2/2560 (0.1%)
2	H	0.84	0/1872	0.88	3/2538 (0.1%)
2	J	0.79	0/1892	0.84	1/2566 (0.0%)
2	L	0.74	0/1886	0.84	2/2558 (0.1%)
2	N	0.80	1/1892 (0.1%)	0.85	0/2566
2	P	0.72	0/1882	0.84	2/2553 (0.1%)
2	R	0.71	0/1851	0.83	1/2510 (0.0%)
2	T	0.82	0/1883	0.84	0/2554
2	V	0.82	0/1872	0.86	0/2539
2	X	0.80	0/1877	0.85	1/2546 (0.0%)
2	Z	0.79	0/1846	0.86	1/2503 (0.0%)
All	All	0.75	2/50492 (0.0%)	0.84	31/68366 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	446	ALA	CA-CB	-5.78	1.40	1.52
2	N	313	VAL	CB-CG1	-5.39	1.41	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	213	LEU	N-CA-C	-5.97	94.87	111.00
1	S	213	LEU	N-CA-C	-5.95	94.93	111.00
1	Y	213	LEU	N-CA-C	-5.92	95.00	111.00
2	L	488	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	I	213	LEU	N-CA-C	-5.86	95.19	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1693	0	1688	133	0
1	A	1713	0	1713	132	0
1	B	1695	0	1685	124	0
1	D	1717	0	1712	138	0
1	F	1706	0	1705	89	0
1	I	1680	0	1673	99	0
1	K	1705	0	1702	149	0
1	M	1730	0	1726	112	0
1	O	1675	0	1676	104	0
1	Q	1716	0	1710	145	0
1	S	1686	0	1685	102	0
1	U	1706	0	1705	150	0
1	W	1710	0	1705	125	0
1	Y	1730	0	1726	91	0
2	2	1829	0	1824	64	0
2	C	1853	0	1850	104	0
2	E	1834	0	1829	94	0
2	G	1858	0	1855	76	0
2	H	1844	0	1841	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1863	0	1858	85	0
2	L	1857	0	1853	101	0
2	N	1863	0	1858	73	0
2	P	1853	0	1850	98	0
2	R	1822	0	1815	84	0
2	T	1854	0	1850	74	0
2	V	1843	0	1837	73	0
2	X	1848	0	1845	95	0
2	Z	1817	0	1810	82	0
3	1	3	0	0	3	0
3	2	5	0	0	0	0
3	A	6	0	0	3	0
3	B	2	0	0	0	0
3	C	3	0	0	1	0
3	D	3	0	0	1	0
3	E	1	0	0	0	0
3	F	4	0	0	1	0
3	G	13	0	0	0	0
3	H	3	0	0	1	0
3	I	2	0	0	1	0
3	J	3	0	0	1	0
3	K	4	0	0	0	0
3	L	2	0	0	1	0
3	M	5	0	0	5	0
3	N	4	0	0	0	0
3	O	1	0	0	1	0
3	P	5	0	0	0	0
3	R	1	0	0	0	0
3	S	3	0	0	0	0
3	T	3	0	0	0	0
3	U	2	0	0	0	0
3	V	4	0	0	1	0
3	W	6	0	0	0	0
3	X	2	0	0	0	0
3	Y	6	0	0	1	0
3	Z	5	0	0	0	0
All	All	49801	0	49586	2615	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 26.

The worst 5 of 2615 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:35:TYR:CE1	1:Q:37:GLY:HA3	1.51	1.43
1:O:35:TYR:CE1	1:O:37:GLY:HA3	1.56	1.40
2:H:407:TYR:CE1	2:H:417:ALA:HB3	1.59	1.36
1:S:35:TYR:CE1	1:S:37:GLY:HA3	1.56	1.36
1:B:35:TYR:CE1	1:B:37:GLY:HA3	1.60	1.35

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	1	215/248 (87%)	204 (95%)	10 (5%)	1 (0%)	34 55
1	A	218/248 (88%)	208 (95%)	10 (5%)	0	100 100
1	B	216/248 (87%)	205 (95%)	11 (5%)	0	100 100
1	D	218/248 (88%)	202 (93%)	16 (7%)	0	100 100
1	F	217/248 (88%)	208 (96%)	9 (4%)	0	100 100
1	I	213/248 (86%)	204 (96%)	9 (4%)	0	100 100
1	K	217/248 (88%)	206 (95%)	11 (5%)	0	100 100
1	M	220/248 (89%)	215 (98%)	5 (2%)	0	100 100
1	O	214/248 (86%)	202 (94%)	12 (6%)	0	100 100
1	Q	218/248 (88%)	205 (94%)	13 (6%)	0	100 100
1	S	215/248 (87%)	202 (94%)	13 (6%)	0	100 100
1	U	217/248 (88%)	203 (94%)	14 (6%)	0	100 100
1	W	217/248 (88%)	205 (94%)	11 (5%)	1 (0%)	34 55
1	Y	220/248 (89%)	212 (96%)	8 (4%)	0	100 100
2	2	242/291 (83%)	241 (100%)	1 (0%)	0	100 100
2	C	246/291 (84%)	241 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	244/291 (84%)	239 (98%)	5 (2%)	0	100	100
2	G	247/291 (85%)	246 (100%)	1 (0%)	0	100	100
2	H	244/291 (84%)	239 (98%)	5 (2%)	0	100	100
2	J	248/291 (85%)	245 (99%)	3 (1%)	0	100	100
2	L	247/291 (85%)	240 (97%)	6 (2%)	1 (0%)	39	61
2	N	248/291 (85%)	244 (98%)	4 (2%)	0	100	100
2	P	246/291 (84%)	244 (99%)	2 (1%)	0	100	100
2	R	242/291 (83%)	240 (99%)	2 (1%)	0	100	100
2	T	246/291 (84%)	243 (99%)	3 (1%)	0	100	100
2	V	245/291 (84%)	244 (100%)	1 (0%)	0	100	100
2	X	245/291 (84%)	244 (100%)	1 (0%)	0	100	100
2	Z	241/291 (83%)	240 (100%)	1 (0%)	0	100	100
All	All	6466/7546 (86%)	6271 (97%)	192 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	4	PRO
2	L	-19	ALA
1	1	7	ILE

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	1	168/192 (88%)	150 (89%)	18 (11%)	8	15
1	A	171/192 (89%)	157 (92%)	14 (8%)	14	27
1	B	168/192 (88%)	152 (90%)	16 (10%)	11	20
1	D	171/192 (89%)	157 (92%)	14 (8%)	14	27
1	F	170/192 (88%)	155 (91%)	15 (9%)	12	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	167/192 (87%)	151 (90%)	16 (10%)	10	19
1	K	170/192 (88%)	154 (91%)	16 (9%)	11	20
1	M	173/192 (90%)	157 (91%)	16 (9%)	11	21
1	O	167/192 (87%)	153 (92%)	14 (8%)	14	25
1	Q	171/192 (89%)	152 (89%)	19 (11%)	8	14
1	S	168/192 (88%)	154 (92%)	14 (8%)	14	26
1	U	170/192 (88%)	153 (90%)	17 (10%)	9	18
1	W	170/192 (88%)	153 (90%)	17 (10%)	9	18
1	Y	173/192 (90%)	155 (90%)	18 (10%)	9	16
2	2	186/216 (86%)	175 (94%)	11 (6%)	24	44
2	C	188/216 (87%)	176 (94%)	12 (6%)	22	39
2	E	185/216 (86%)	168 (91%)	17 (9%)	11	21
2	G	188/216 (87%)	177 (94%)	11 (6%)	24	44
2	H	186/216 (86%)	178 (96%)	8 (4%)	35	61
2	J	189/216 (88%)	179 (95%)	10 (5%)	28	50
2	L	188/216 (87%)	175 (93%)	13 (7%)	19	35
2	N	189/216 (88%)	178 (94%)	11 (6%)	25	45
2	P	188/216 (87%)	174 (93%)	14 (7%)	17	31
2	R	184/216 (85%)	175 (95%)	9 (5%)	31	55
2	T	189/216 (88%)	176 (93%)	13 (7%)	19	35
2	V	186/216 (86%)	178 (96%)	8 (4%)	35	61
2	X	188/216 (87%)	173 (92%)	15 (8%)	15	28
2	Z	184/216 (85%)	169 (92%)	15 (8%)	14	27
All	All	4995/5712 (87%)	4604 (92%)	391 (8%)	16	29

5 of 391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	208	LEU
1	Q	5	TYR
2	Z	520	SER
2	N	329	ARG
1	O	122	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	73	ASN
1	Q	51	GLN
2	2	-5	GLN
1	M	105	GLN
1	O	69	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	219/248 (88%)	0.77	33 (15%) 3 3	48, 86, 121, 152	0
1	A	222/248 (89%)	0.30	13 (5%) 26 29	43, 81, 117, 145	0
1	B	220/248 (88%)	0.47	17 (7%) 16 18	48, 88, 127, 145	0
1	D	222/248 (89%)	0.48	20 (9%) 12 12	52, 92, 126, 144	0
1	F	221/248 (89%)	0.56	24 (10%) 7 7	45, 86, 126, 147	0
1	I	217/248 (87%)	0.35	16 (7%) 17 19	45, 80, 123, 149	0
1	K	221/248 (89%)	0.90	39 (17%) 2 2	48, 98, 135, 148	0
1	M	224/248 (90%)	0.35	13 (5%) 26 30	45, 78, 127, 147	0
1	O	218/248 (87%)	0.68	26 (11%) 6 6	50, 97, 137, 150	0
1	Q	222/248 (89%)	0.57	19 (8%) 13 14	48, 96, 131, 140	0
1	S	219/248 (88%)	0.58	20 (9%) 11 12	46, 85, 129, 140	0
1	U	221/248 (89%)	0.45	17 (7%) 16 18	49, 88, 130, 144	0
1	W	221/248 (89%)	0.58	21 (9%) 10 11	48, 81, 125, 149	0
1	Y	224/248 (90%)	0.48	19 (8%) 13 14	53, 93, 132, 142	0
2	2	246/291 (84%)	0.15	10 (4%) 41 46	48, 68, 97, 107	0
2	C	250/291 (85%)	0.19	11 (4%) 38 43	51, 73, 111, 143	0
2	E	248/291 (85%)	0.28	16 (6%) 22 25	30, 77, 115, 132	0
2	G	251/291 (86%)	0.08	5 (1%) 68 72	45, 67, 115, 141	0
2	H	249/291 (85%)	0.26	14 (5%) 28 31	45, 71, 113, 136	0
2	J	252/291 (86%)	0.15	11 (4%) 38 43	47, 70, 109, 135	0
2	L	251/291 (86%)	0.19	8 (3%) 51 56	51, 75, 116, 140	0
2	N	252/291 (86%)	0.18	8 (3%) 51 56	44, 70, 115, 144	0
2	P	250/291 (85%)	0.24	10 (4%) 42 47	47, 75, 114, 144	0
2	R	246/291 (84%)	0.22	10 (4%) 41 46	30, 82, 118, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	T	250/291 (85%)	0.03	5 (2%) 68 72	40, 68, 110, 137	0
2	V	249/291 (85%)	-0.07	3 (1%) 81 83	47, 68, 112, 136	0
2	X	249/291 (85%)	0.17	11 (4%) 38 43	44, 65, 115, 144	0
2	Z	245/291 (84%)	0.11	8 (3%) 50 55	49, 73, 115, 131	0
All	All	6579/7546 (87%)	0.33	427 (6%) 22 25	30, 78, 124, 152	0

The worst 5 of 427 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	5	TYR	12.1
1	U	5	TYR	10.3
1	1	6	PHE	9.6
1	W	4	PRO	8.0
1	K	7	ILE	7.9

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.