



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:11 PM BST

PDB ID : 3C92
EMDB ID: : EMD-1740
Title : Thermoplasma acidophilum 20S proteasome with a closed gate
Authors : Rabl, J.; Smith, D.M.; Yu, Y.; Chang, S.C.; Goldberg, A.L.; Cheng, Y.
Deposited on : 2008-02-14
Resolution : 6.80 Å(reported)
Based on PDB ID : 1PMA 3C91

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

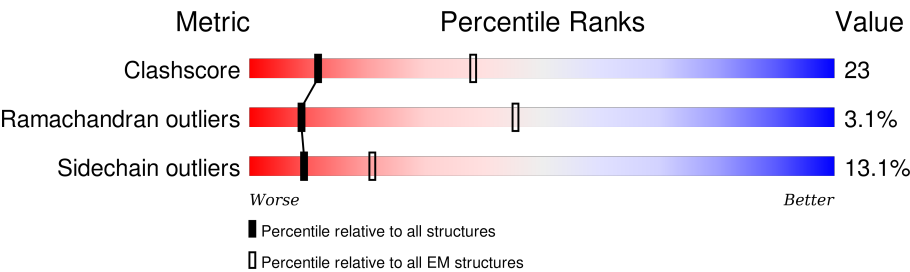
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 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.






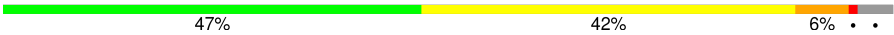















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	233	48% 41% 6% . .
1	B	233	48% 42% 6% . .
1	C	233	47% 42% 6% . .
1	D	233	48% 41% 6% . .
1	E	233	46% 43% 6% . .
1	F	233	48% 41% 6% . .
1	G	233	48% 40% 6% . .
1	O	233	48% 41% 6% . .
1	P	233	48% 42% 6% . .

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Mol	Chain	Length	Quality of chain
1	Q	233	
1	R	233	
1	S	233	
1	T	233	
1	U	233	
2	1	203	
2	2	203	
2	H	203	
2	I	203	
2	J	203	
2	K	203	
2	L	203	
2	M	203	
2	N	203	
2	V	203	
2	W	203	
2	X	203	
2	Y	203	
2	Z	203	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 46228 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	B	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	C	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	D	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	E	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	F	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	G	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	O	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	P	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	Q	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	R	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	S	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	T	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	U	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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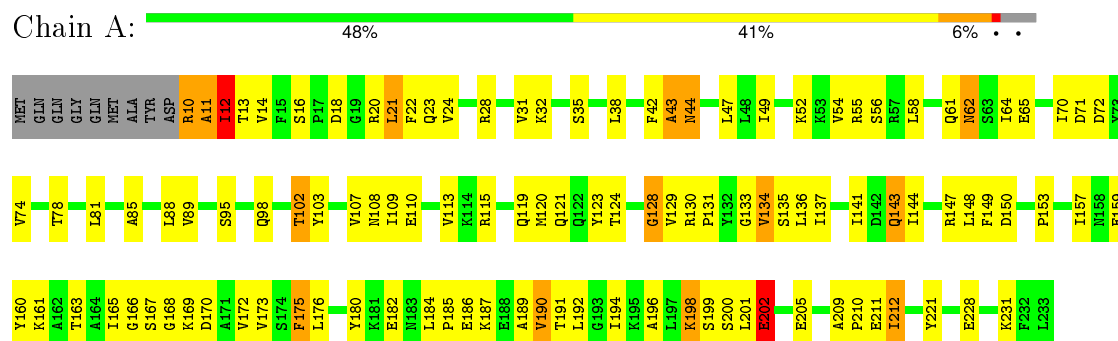
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	K	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	M	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	W	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	Y	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

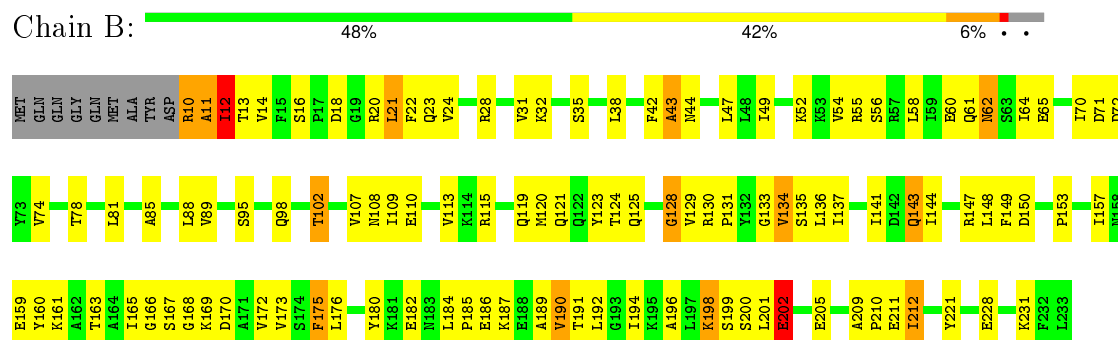
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

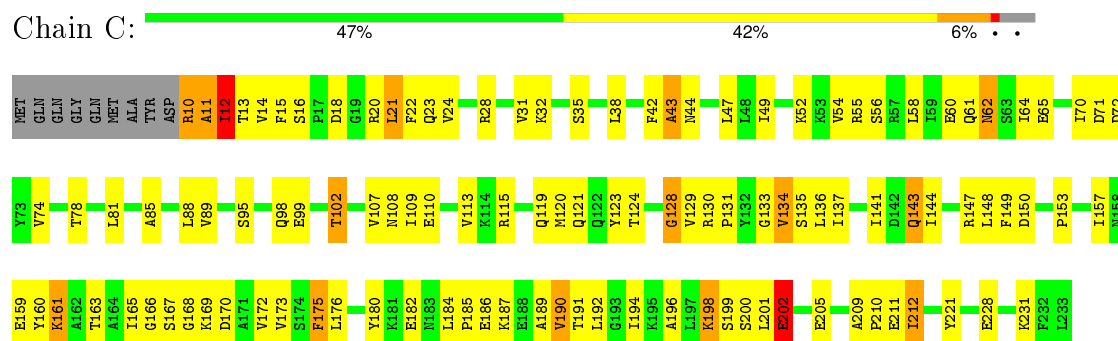
- Molecule 1: Proteasome subunit alpha



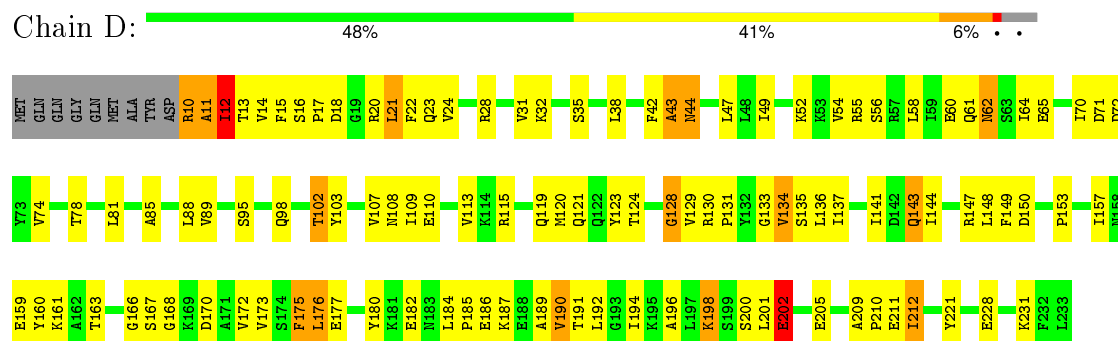
- Molecule 1: Proteasome subunit alpha



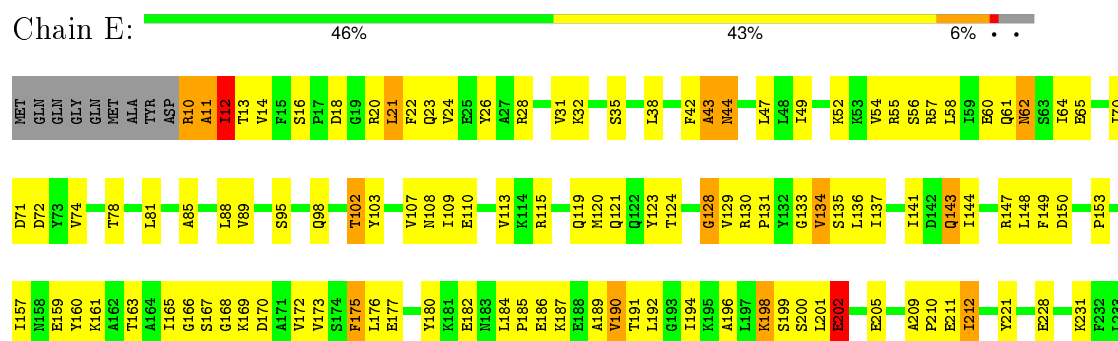
- Molecule 1: Proteasome subunit alpha



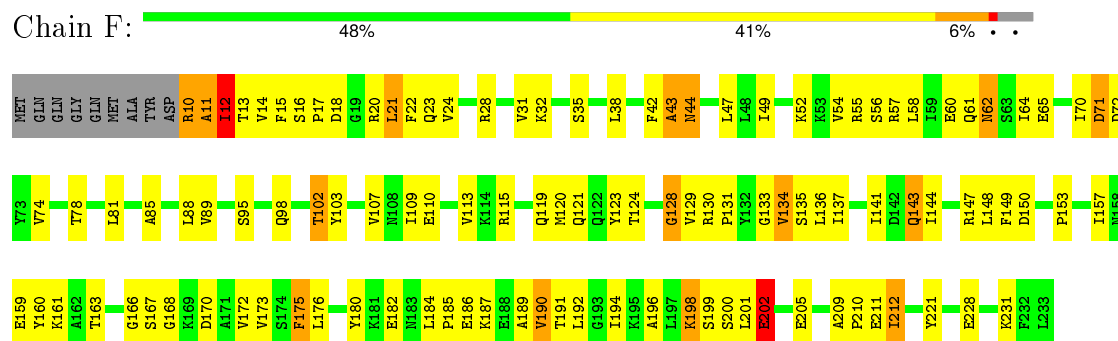
- Molecule 1: Proteasome subunit alpha



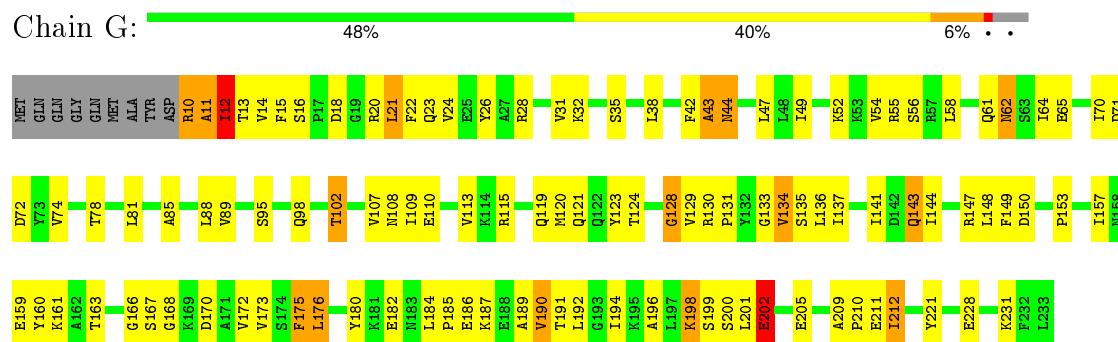
- Molecule 1: Proteasome subunit alpha



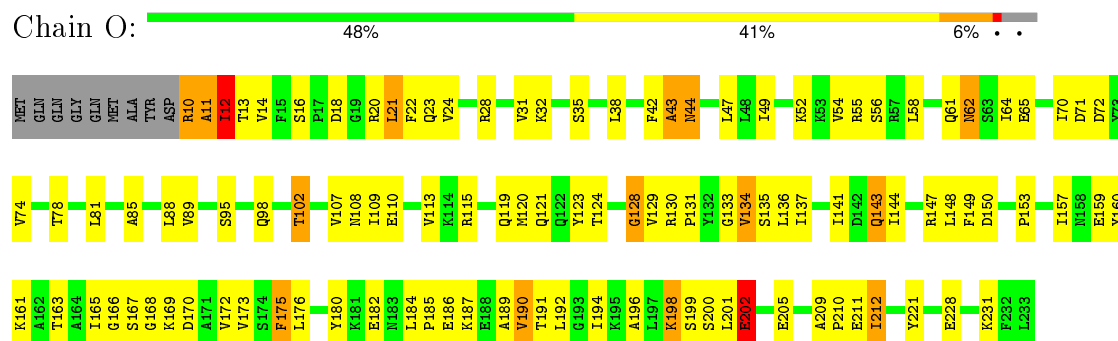
- Molecule 1: Proteasome subunit alpha



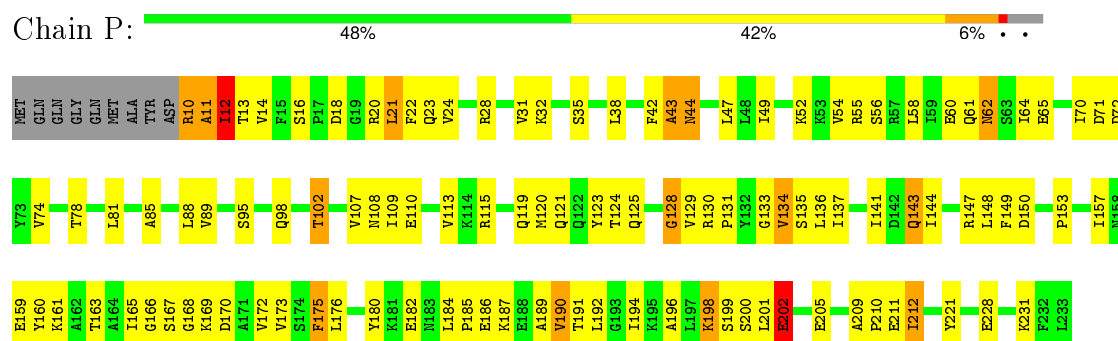
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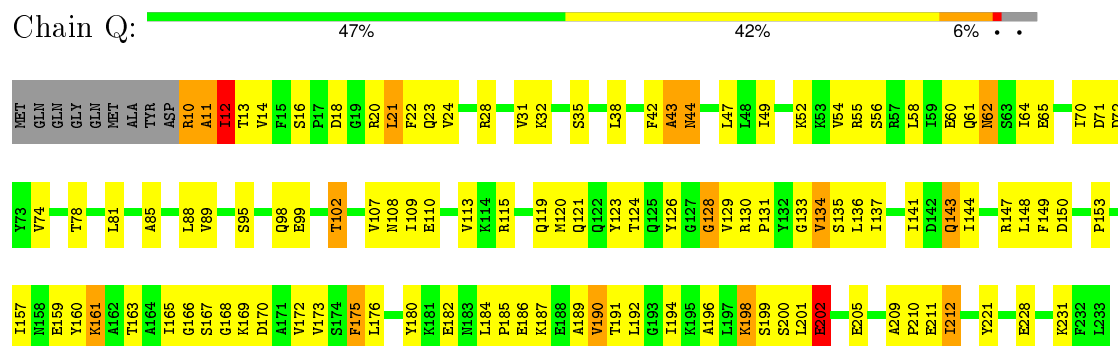
- Molecule 1: Proteasome subunit alpha



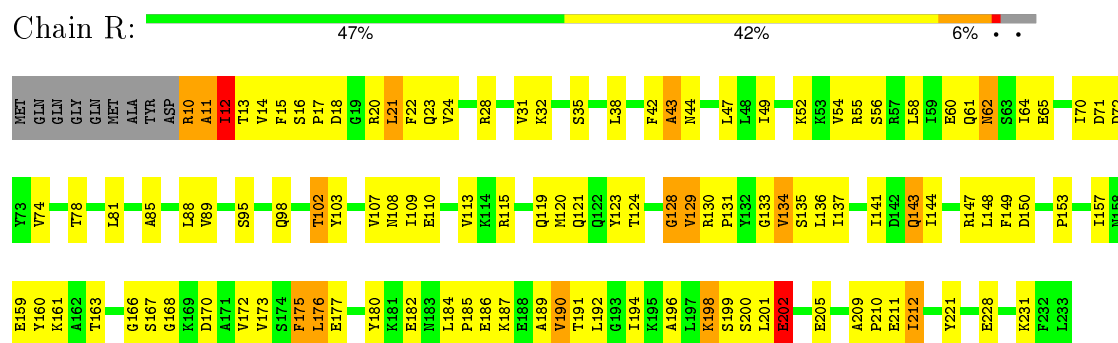
- Molecule 1: Proteasome subunit alpha



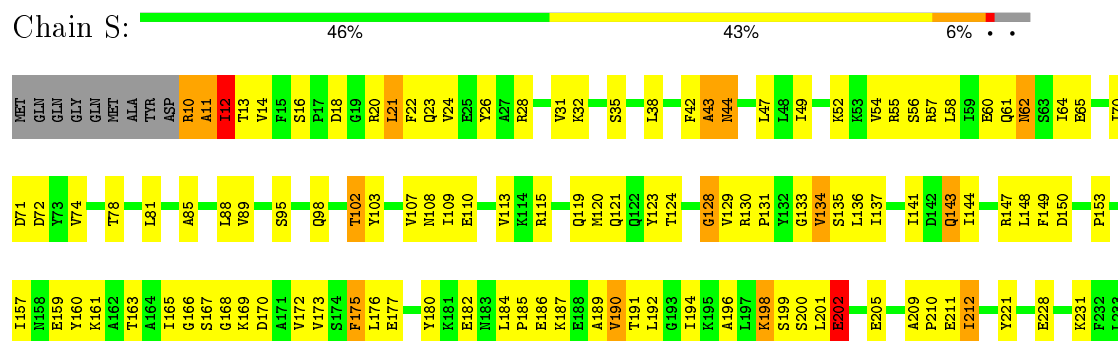
- Molecule 1: Proteasome subunit alpha



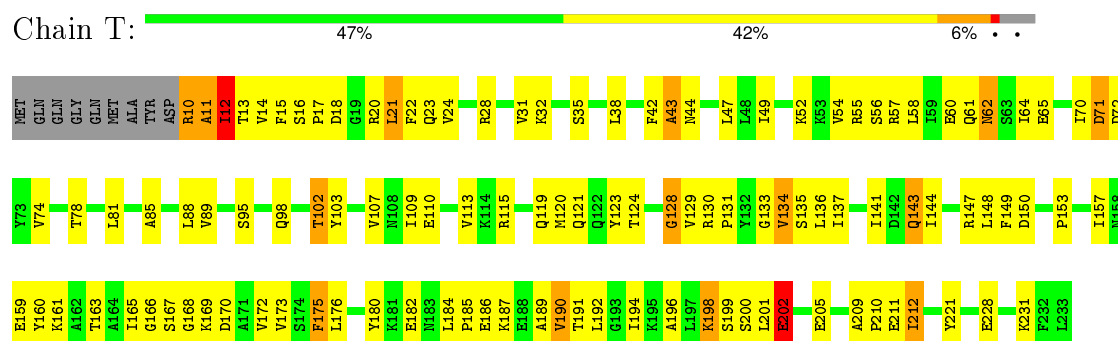
- Molecule 1: Proteasome subunit alpha



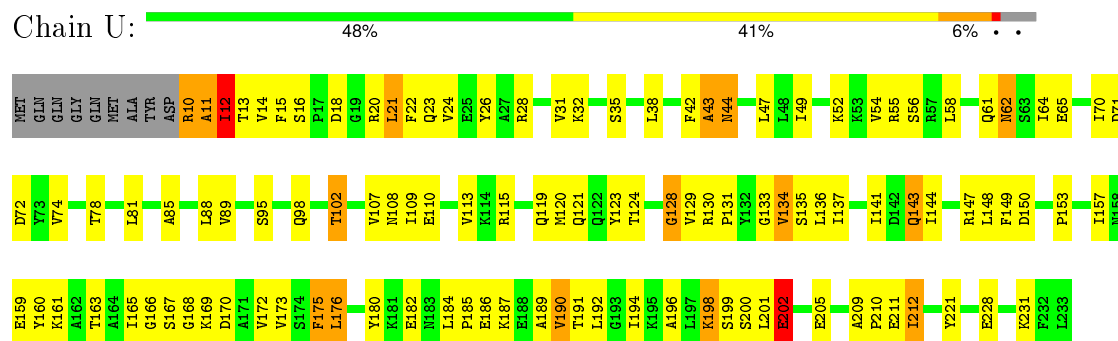
- Molecule 1: Proteasome subunit alpha



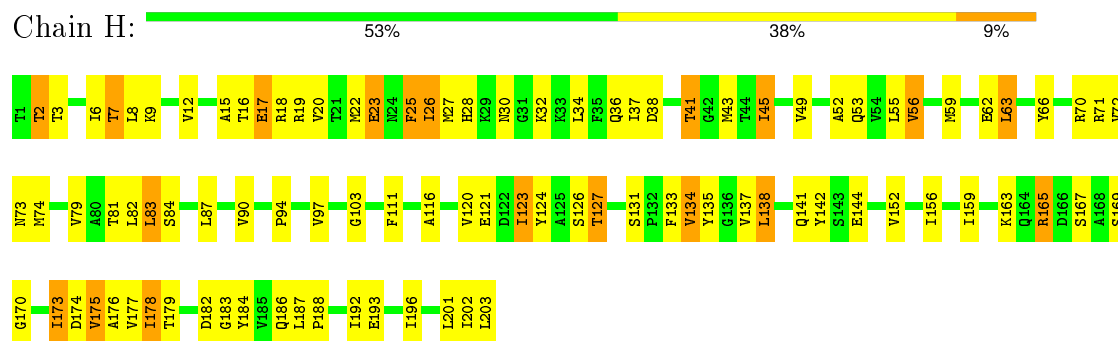
- Molecule 1: Proteasome subunit alpha



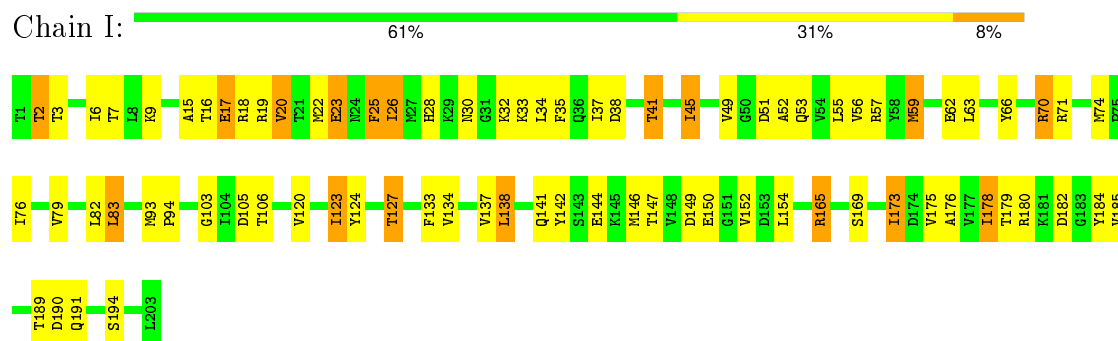
- Molecule 1: Proteasome subunit alpha



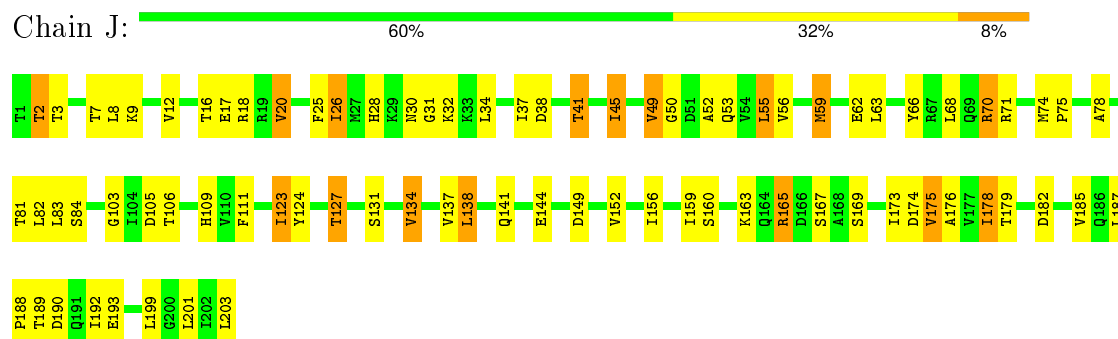
- Molecule 2: Proteasome subunit beta



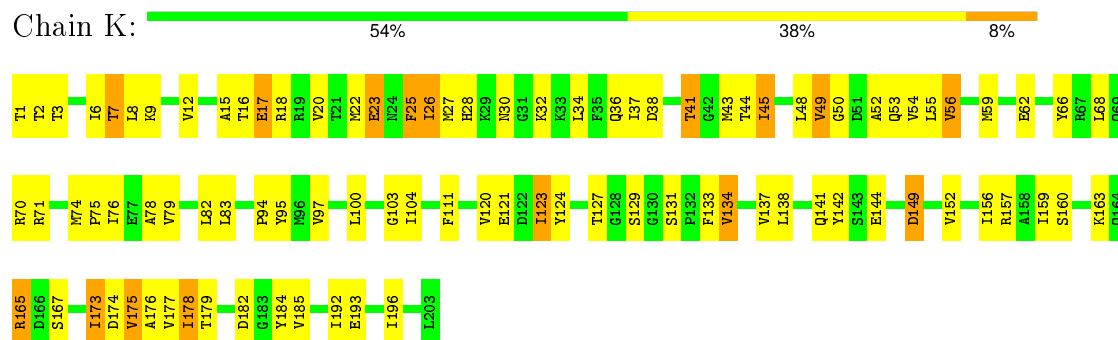
- Molecule 2: Proteasome subunit beta



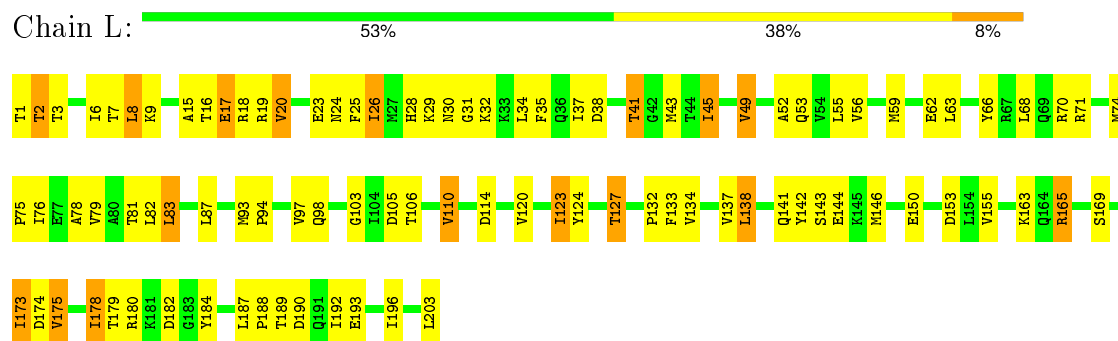
- Molecule 2: Proteasome subunit beta



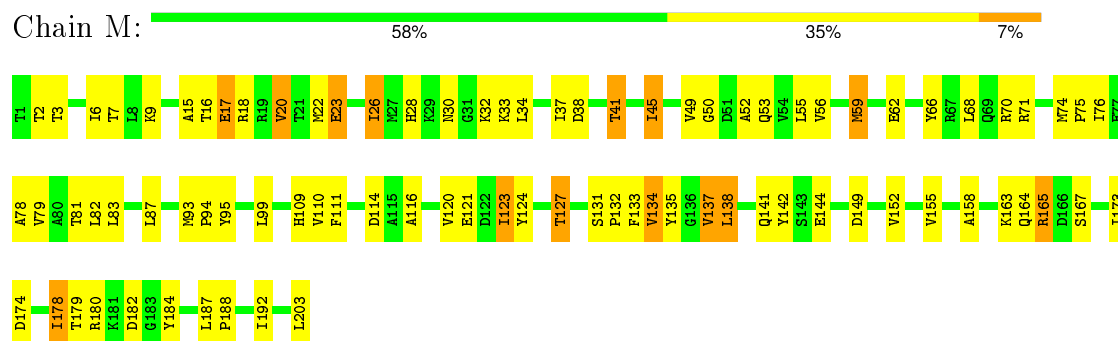
- Molecule 2: Proteasome subunit beta

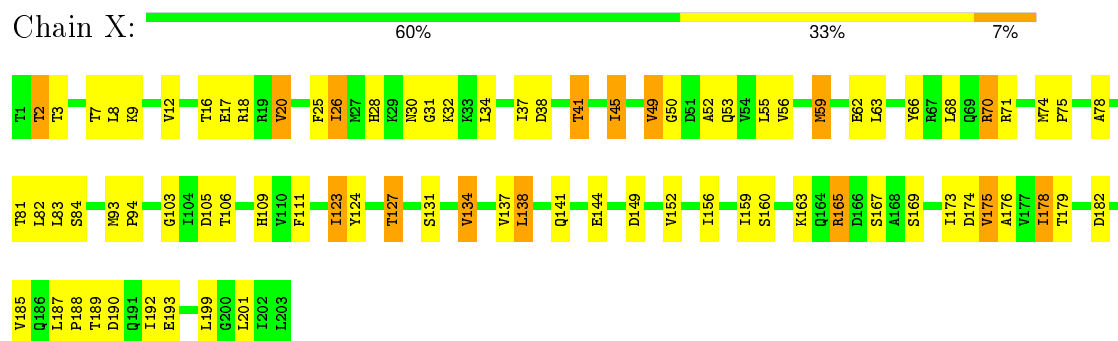


- Molecule 2: Proteasome subunit beta

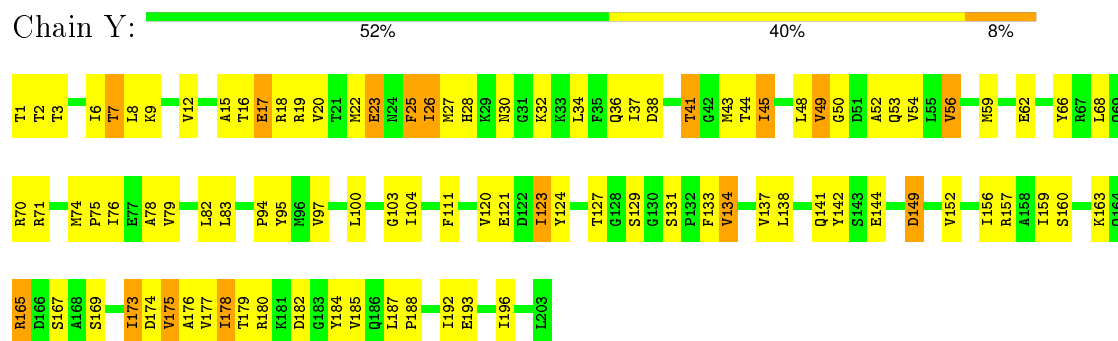


- Molecule 2: Proteasome subunit beta

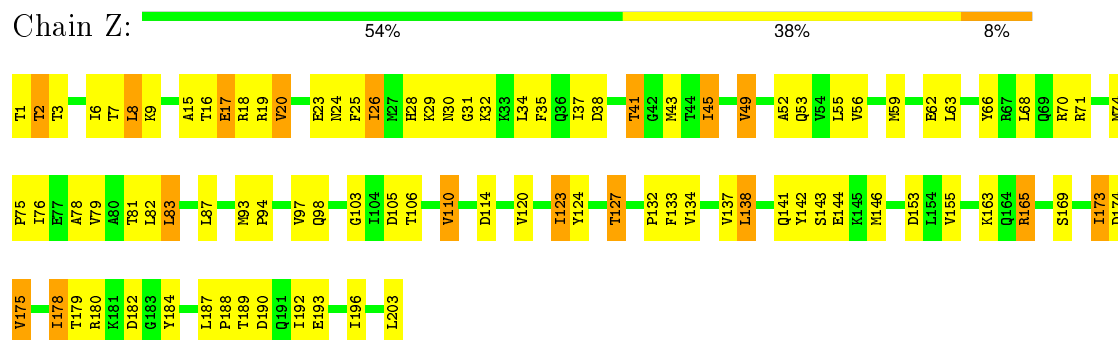




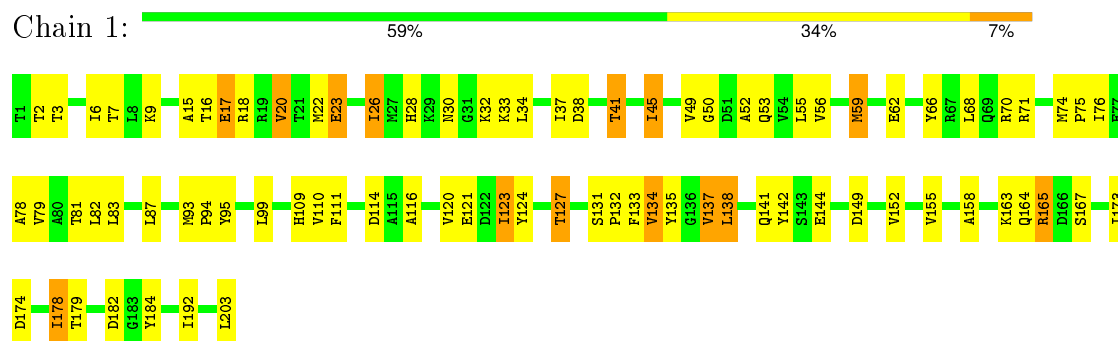
- Molecule 2: Proteasome subunit beta



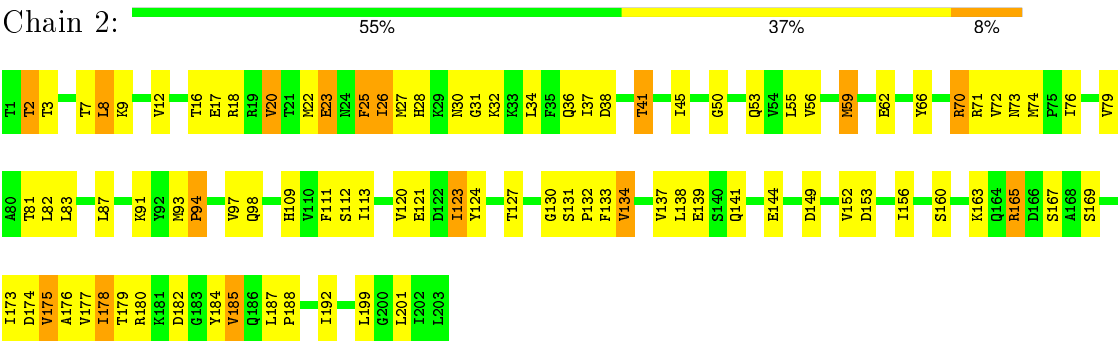
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE AND AMPLITUDE	Depositor
Microscope	FEI TECNAI TF20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2000.00	Depositor
Minimum defocus (nm)	-1500.00	Depositor
Maximum defocus (nm)	-3500.00	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.55	0/1767	0.81	6/2380 (0.3%)
1	B	0.55	0/1767	0.81	6/2380 (0.3%)
1	C	0.55	0/1767	0.81	6/2380 (0.3%)
1	D	0.55	0/1767	0.81	6/2380 (0.3%)
1	E	0.55	0/1767	0.81	6/2380 (0.3%)
1	F	0.56	0/1767	0.81	6/2380 (0.3%)
1	G	0.56	0/1767	0.81	6/2380 (0.3%)
1	O	0.55	0/1767	0.81	6/2380 (0.3%)
1	P	0.56	0/1767	0.81	6/2380 (0.3%)
1	Q	0.56	0/1767	0.81	6/2380 (0.3%)
1	R	0.55	0/1767	0.81	6/2380 (0.3%)
1	S	0.55	0/1767	0.81	6/2380 (0.3%)
1	T	0.56	0/1767	0.82	6/2380 (0.3%)
1	U	0.56	0/1767	0.81	6/2380 (0.3%)
2	1	0.55	0/1577	0.75	1/2129 (0.0%)
2	2	0.54	0/1577	0.75	0/2129
2	H	0.57	0/1577	0.76	0/2129
2	I	0.57	0/1577	0.76	0/2129
2	J	0.54	0/1577	0.75	0/2129
2	K	0.55	0/1577	0.77	2/2129 (0.1%)
2	L	0.57	0/1577	0.77	0/2129
2	M	0.55	0/1577	0.75	1/2129 (0.0%)
2	N	0.54	0/1577	0.75	0/2129
2	V	0.57	0/1577	0.76	0/2129
2	W	0.57	0/1577	0.76	0/2129
2	X	0.54	0/1577	0.75	0/2129
2	Y	0.55	0/1577	0.77	2/2129 (0.1%)
2	Z	0.57	0/1577	0.77	0/2129
All	All	0.56	0/46816	0.79	90/63126 (0.1%)

There are no bond length outliers.

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	12	ILE	CB-CA-C	-10.42	90.76	111.60
1	T	12	ILE	CB-CA-C	-10.41	90.79	111.60
1	C	12	ILE	CB-CA-C	-10.40	90.79	111.60
1	G	12	ILE	CB-CA-C	-10.40	90.79	111.60
1	U	12	ILE	CB-CA-C	-10.40	90.80	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1744	0	1781	93	0
1	B	1744	0	1781	90	0
1	C	1744	0	1781	91	0
1	D	1744	0	1781	95	0
1	E	1744	0	1781	100	0
1	F	1744	0	1781	93	0
1	G	1744	0	1781	95	0
1	O	1744	0	1781	91	0
1	P	1744	0	1781	91	0
1	Q	1744	0	1781	93	0
1	R	1744	0	1781	97	0
1	S	1744	0	1781	100	0
1	T	1744	0	1781	95	0
1	U	1744	0	1781	94	0
2	1	1558	0	1609	80	0
2	2	1558	0	1609	74	0
2	H	1558	0	1609	81	0
2	I	1558	0	1609	62	0
2	J	1558	0	1609	65	0
2	K	1558	0	1609	71	0
2	L	1558	0	1609	86	0
2	M	1558	0	1609	81	0
2	N	1558	0	1609	75	0
2	V	1558	0	1609	83	0
2	W	1558	0	1609	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	1558	0	1609	57	0
2	Y	1558	0	1609	74	0
2	Z	1558	0	1609	82	0
All	All	46228	0	47460	2137	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 23.

The worst 5 of 2137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:ILE:HG21	1:D:14:VAL:CG2	1.50	1.41
1:E:12:ILE:HG21	1:E:14:VAL:CG2	1.50	1.40
1:C:12:ILE:HG21	1:C:14:VAL:CG2	1.50	1.39
1:O:12:ILE:HG21	1:O:14:VAL:CG2	1.50	1.39
1:P:12:ILE:HG21	1:P:14:VAL:CG2	1.50	1.39

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	B	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	C	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	D	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	E	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	F	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	G	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	P	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	Q	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	R	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	S	222/233 (95%)	183 (82%)	28 (13%)	11 (5%)	3	31
1	T	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
1	U	222/233 (95%)	184 (83%)	27 (12%)	11 (5%)	3	31
2	1	201/203 (99%)	176 (88%)	23 (11%)	2 (1%)	19	65
2	2	201/203 (99%)	184 (92%)	15 (8%)	2 (1%)	19	65
2	H	201/203 (99%)	184 (92%)	15 (8%)	2 (1%)	19	65
2	I	201/203 (99%)	183 (91%)	16 (8%)	2 (1%)	19	65
2	J	201/203 (99%)	180 (90%)	20 (10%)	1 (0%)	34	77
2	K	201/203 (99%)	184 (92%)	15 (8%)	2 (1%)	19	65
2	L	201/203 (99%)	181 (90%)	16 (8%)	4 (2%)	9	51
2	M	201/203 (99%)	176 (88%)	23 (11%)	2 (1%)	19	65
2	N	201/203 (99%)	184 (92%)	15 (8%)	2 (1%)	19	65
2	V	201/203 (99%)	185 (92%)	14 (7%)	2 (1%)	19	65
2	W	201/203 (99%)	183 (91%)	16 (8%)	2 (1%)	19	65
2	X	201/203 (99%)	180 (90%)	20 (10%)	1 (0%)	34	77
2	Y	201/203 (99%)	184 (92%)	15 (8%)	2 (1%)	19	65
2	Z	201/203 (99%)	181 (90%)	16 (8%)	4 (2%)	9	51
All	All	5922/6104 (97%)	5120 (86%)	618 (10%)	184 (3%)	9	42

5 of 184 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	128	GLY
1	A	182	GLU
1	A	200	SER
1	B	12	ILE

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 PDB entries followed by that with respect to all EM entries.

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	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	B	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	C	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	D	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	E	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	F	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	G	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	O	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	P	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	Q	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	R	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	S	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	T	186/193 (96%)	163 (88%)	23 (12%)	6	30
1	U	186/193 (96%)	163 (88%)	23 (12%)	6	30
2	1	170/170 (100%)	152 (89%)	18 (11%)	8	36
2	2	170/170 (100%)	146 (86%)	24 (14%)	4	26
2	H	170/170 (100%)	145 (85%)	25 (15%)	4	24
2	I	170/170 (100%)	148 (87%)	22 (13%)	5	28
2	J	170/170 (100%)	143 (84%)	27 (16%)	3	21
2	K	170/170 (100%)	143 (84%)	27 (16%)	3	21
2	L	170/170 (100%)	146 (86%)	24 (14%)	4	26
2	M	170/170 (100%)	152 (89%)	18 (11%)	8	36
2	N	170/170 (100%)	146 (86%)	24 (14%)	4	26
2	V	170/170 (100%)	145 (85%)	25 (15%)	4	24
2	W	170/170 (100%)	149 (88%)	21 (12%)	6	30
2	X	170/170 (100%)	143 (84%)	27 (16%)	3	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Y	170/170 (100%)	143 (84%)	27 (16%)	3	21
2	Z	170/170 (100%)	146 (86%)	24 (14%)	4	26
All	All	4984/5082 (98%)	4329 (87%)	655 (13%)	9	28

5 of 655 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	127	THR
1	P	161	LYS
2	Z	137	VAL
2	N	8	LEU
1	O	44	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	141	GLN
1	P	23	GLN
2	Y	85	ASN
2	M	30	ASN
1	O	23	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.