



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 06:34 PM EDT

PDB ID : 3IPM / pdb\_00003ipm  
Title : Crystal Structure of Archaeal 20S Proteasome in Complex with the C-terminus of PAN  
Authors : Yu, Y.; Cheng, Y.  
Deposited on : 2009-08-17  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

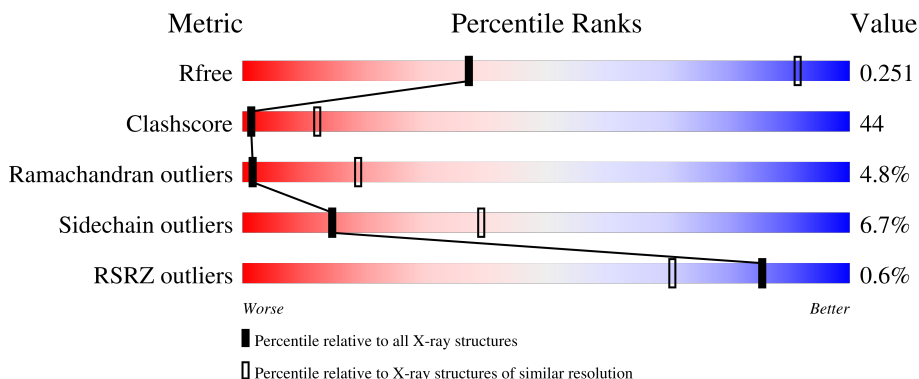
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	233	
1	B	233	
1	C	233	
1	D	233	
1	E	233	

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Mol	Chain	Length	Quality of chain
1	F	233	 28% 59% 9% . .
1	G	233	 29% 58% 9% . .
2	H	217	 % 37% 49% 7% 6%
2	I	217	 % 38% 46% 9% 6%
2	J	217	 41% 44% 8% 6%
2	K	217	 40% 45% 9% 6%
2	L	217	 40% 45% 9% 6%
2	M	217	 2% 38% 45% 10% 6%
2	N	217	 % 38% 47% 8% 6%
3	O	239	 40% 46% 6% 8%
3	P	239	 37% 49% 5% 8%
3	Q	239	 39% 46% 6% 8%
3	R	239	 38% 48% 5% 8%
3	S	239	 38% 48% 5% 8%
3	T	239	 37% 50% 5% 8%
3	U	239	 41% 46% 5% 8%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35133 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
			Total	C	N	O	S			
1	A	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	B	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	C	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	D	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	E	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	F	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0
1	G	227	Total 1769	C 1123	N 299	O 344	S 3	0	0	0

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	I	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	J	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	K	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	L	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	M	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0
2	N	203	Total 1557	C 985	N 264	O 297	S 11	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	204	HIS	-	expression tag	UNP P28061
H	205	HIS	-	expression tag	UNP P28061
H	206	HIS	-	expression tag	UNP P28061
H	207	HIS	-	expression tag	UNP P28061
H	208	HIS	-	expression tag	UNP P28061
H	209	HIS	-	expression tag	UNP P28061
I	204	HIS	-	expression tag	UNP P28061
I	205	HIS	-	expression tag	UNP P28061
I	206	HIS	-	expression tag	UNP P28061
I	207	HIS	-	expression tag	UNP P28061
I	208	HIS	-	expression tag	UNP P28061
I	209	HIS	-	expression tag	UNP P28061
J	204	HIS	-	expression tag	UNP P28061
J	205	HIS	-	expression tag	UNP P28061
J	206	HIS	-	expression tag	UNP P28061
J	207	HIS	-	expression tag	UNP P28061
J	208	HIS	-	expression tag	UNP P28061
J	209	HIS	-	expression tag	UNP P28061
K	204	HIS	-	expression tag	UNP P28061
K	205	HIS	-	expression tag	UNP P28061
K	206	HIS	-	expression tag	UNP P28061
K	207	HIS	-	expression tag	UNP P28061
K	208	HIS	-	expression tag	UNP P28061
K	209	HIS	-	expression tag	UNP P28061
L	204	HIS	-	expression tag	UNP P28061
L	205	HIS	-	expression tag	UNP P28061
L	206	HIS	-	expression tag	UNP P28061
L	207	HIS	-	expression tag	UNP P28061
L	208	HIS	-	expression tag	UNP P28061
L	209	HIS	-	expression tag	UNP P28061
M	204	HIS	-	expression tag	UNP P28061
M	205	HIS	-	expression tag	UNP P28061
M	206	HIS	-	expression tag	UNP P28061
M	207	HIS	-	expression tag	UNP P28061
M	208	HIS	-	expression tag	UNP P28061
M	209	HIS	-	expression tag	UNP P28061
N	204	HIS	-	expression tag	UNP P28061
N	205	HIS	-	expression tag	UNP P28061
N	206	HIS	-	expression tag	UNP P28061
N	207	HIS	-	expression tag	UNP P28061
N	208	HIS	-	expression tag	UNP P28061
N	209	HIS	-	expression tag	UNP P28061

- Molecule 3 is a protein called Proteasome activator PA26, Proteasome-activating nucleotidase fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	O	219	1693	1064	300	324	5	0	0	0
3	P	219	1693	1064	300	324	5	0	0	0
3	Q	219	1693	1064	300	324	5	0	0	0
3	R	219	1693	1064	300	324	5	0	0	0
3	S	219	1693	1064	300	324	5	0	0	0
3	T	219	1693	1064	300	324	5	0	0	0
3	U	219	1693	1064	300	324	5	0	0	0

There are 77 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-6	MET	-	initiating methionine	UNP Q38BM8
O	-5	ALA	-	expression tag	UNP Q38BM8
O	-4	HIS	-	expression tag	UNP Q38BM8
O	-3	HIS	-	expression tag	UNP Q38BM8
O	-2	HIS	-	expression tag	UNP Q38BM8
O	-1	HIS	-	expression tag	UNP Q38BM8
O	0	HIS	-	expression tag	UNP Q38BM8
O	1	HIS	-	expression tag	UNP Q38BM8
O	102	ALA	GLU	engineered mutation	UNP Q38BM8
O	224	GLY	-	linker	UNP Q38BM8
O	225	GLY	-	linker	UNP Q38BM8
P	-6	MET	-	initiating methionine	UNP Q38BM8
P	-5	ALA	-	expression tag	UNP Q38BM8
P	-4	HIS	-	expression tag	UNP Q38BM8
P	-3	HIS	-	expression tag	UNP Q38BM8
P	-2	HIS	-	expression tag	UNP Q38BM8
P	-1	HIS	-	expression tag	UNP Q38BM8
P	0	HIS	-	expression tag	UNP Q38BM8
P	1	HIS	-	expression tag	UNP Q38BM8
P	102	ALA	GLU	engineered mutation	UNP Q38BM8
P	224	GLY	-	linker	UNP Q38BM8
P	225	GLY	-	linker	UNP Q38BM8
Q	-6	MET	-	initiating methionine	UNP Q38BM8

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-5	ALA	-	expression tag	UNP Q38BM8
Q	-4	HIS	-	expression tag	UNP Q38BM8
Q	-3	HIS	-	expression tag	UNP Q38BM8
Q	-2	HIS	-	expression tag	UNP Q38BM8
Q	-1	HIS	-	expression tag	UNP Q38BM8
Q	0	HIS	-	expression tag	UNP Q38BM8
Q	1	HIS	-	expression tag	UNP Q38BM8
Q	102	ALA	GLU	engineered mutation	UNP Q38BM8
Q	224	GLY	-	linker	UNP Q38BM8
Q	225	GLY	-	linker	UNP Q38BM8
R	-6	MET	-	initiating methionine	UNP Q38BM8
R	-5	ALA	-	expression tag	UNP Q38BM8
R	-4	HIS	-	expression tag	UNP Q38BM8
R	-3	HIS	-	expression tag	UNP Q38BM8
R	-2	HIS	-	expression tag	UNP Q38BM8
R	-1	HIS	-	expression tag	UNP Q38BM8
R	0	HIS	-	expression tag	UNP Q38BM8
R	1	HIS	-	expression tag	UNP Q38BM8
R	102	ALA	GLU	engineered mutation	UNP Q38BM8
R	224	GLY	-	linker	UNP Q38BM8
R	225	GLY	-	linker	UNP Q38BM8
S	-6	MET	-	initiating methionine	UNP Q38BM8
S	-5	ALA	-	expression tag	UNP Q38BM8
S	-4	HIS	-	expression tag	UNP Q38BM8
S	-3	HIS	-	expression tag	UNP Q38BM8
S	-2	HIS	-	expression tag	UNP Q38BM8
S	-1	HIS	-	expression tag	UNP Q38BM8
S	0	HIS	-	expression tag	UNP Q38BM8
S	1	HIS	-	expression tag	UNP Q38BM8
S	102	ALA	GLU	engineered mutation	UNP Q38BM8
S	224	GLY	-	linker	UNP Q38BM8
S	225	GLY	-	linker	UNP Q38BM8
T	-6	MET	-	initiating methionine	UNP Q38BM8
T	-5	ALA	-	expression tag	UNP Q38BM8
T	-4	HIS	-	expression tag	UNP Q38BM8
T	-3	HIS	-	expression tag	UNP Q38BM8
T	-2	HIS	-	expression tag	UNP Q38BM8
T	-1	HIS	-	expression tag	UNP Q38BM8
T	0	HIS	-	expression tag	UNP Q38BM8
T	1	HIS	-	expression tag	UNP Q38BM8
T	102	ALA	GLU	engineered mutation	UNP Q38BM8
T	224	GLY	-	linker	UNP Q38BM8

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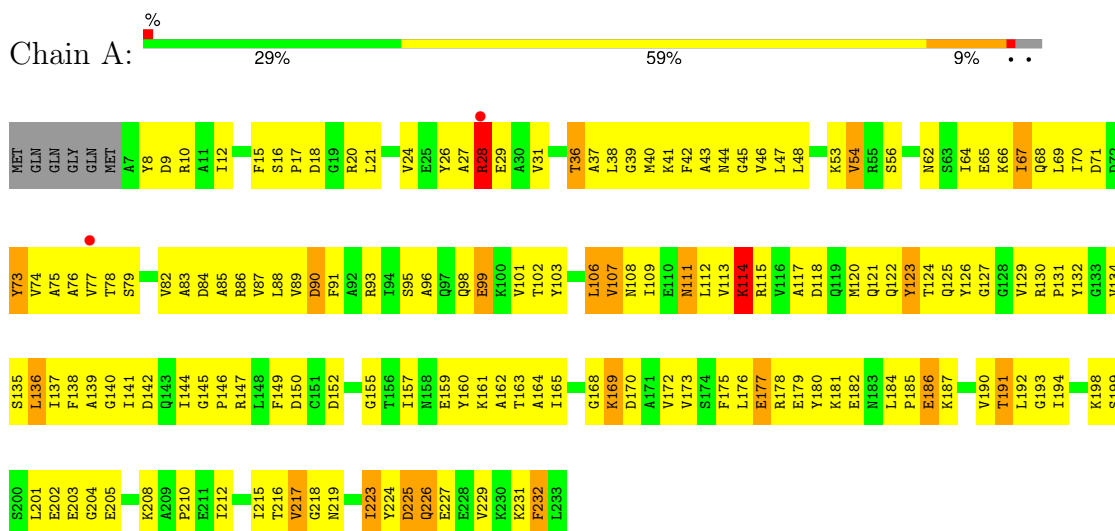
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Chain	Residue	Modelled	Actual	Comment	Reference
T	225	GLY	-	linker	UNP Q38BM8
U	-6	MET	-	initiating methionine	UNP Q38BM8
U	-5	ALA	-	expression tag	UNP Q38BM8
U	-4	HIS	-	expression tag	UNP Q38BM8
U	-3	HIS	-	expression tag	UNP Q38BM8
U	-2	HIS	-	expression tag	UNP Q38BM8
U	-1	HIS	-	expression tag	UNP Q38BM8
U	0	HIS	-	expression tag	UNP Q38BM8
U	1	HIS	-	expression tag	UNP Q38BM8
U	102	ALA	GLU	engineered mutation	UNP Q38BM8
U	224	GLY	-	linker	UNP Q38BM8
U	225	GLY	-	linker	UNP Q38BM8

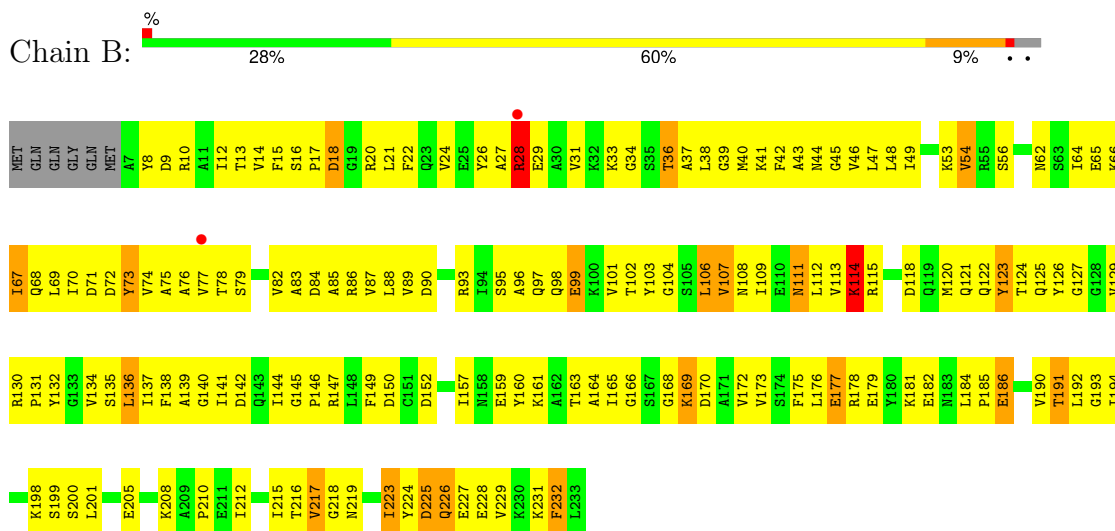
### 3 Residue-property plots

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

- Molecule 1: Proteasome subunit alpha

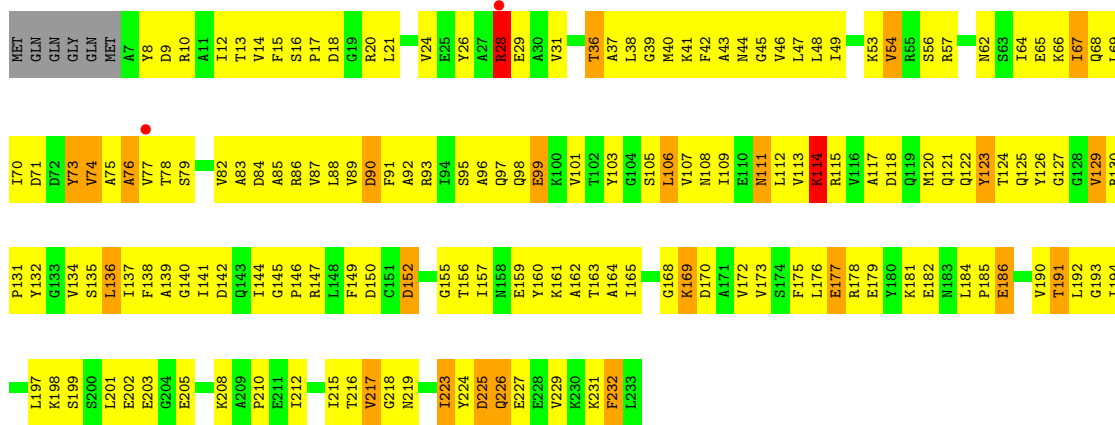


- Molecule 1: Proteasome subunit alpha

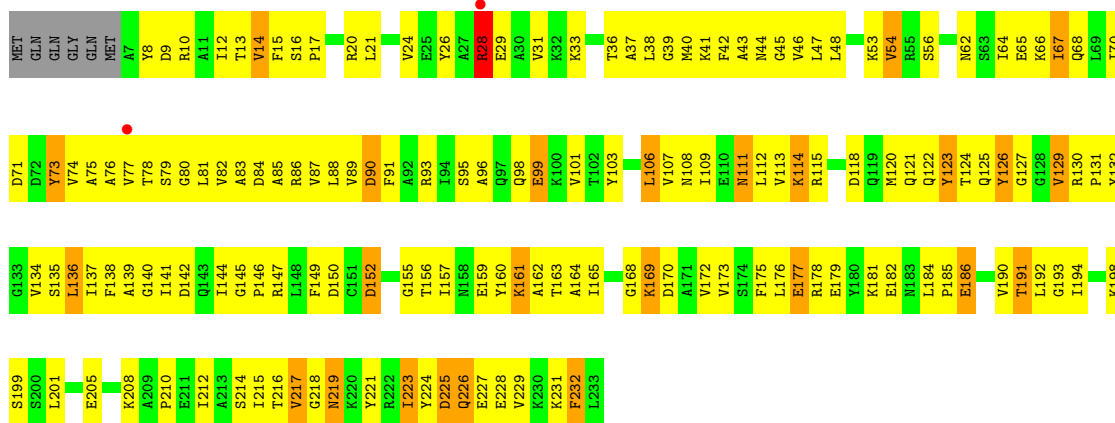


- Molecule 1: Proteasome subunit alpha

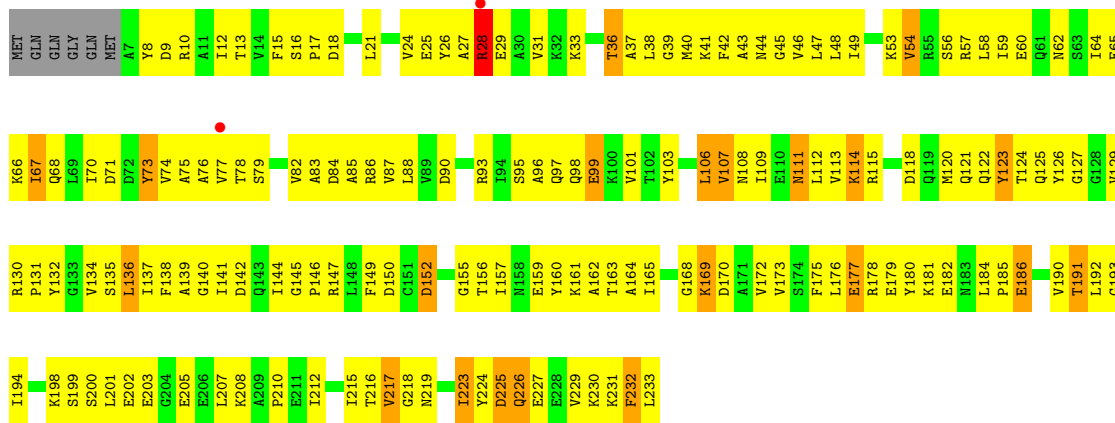




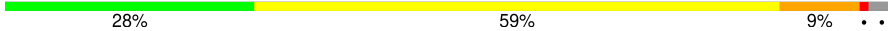
• Molecule 1: Proteasome subunit alpha

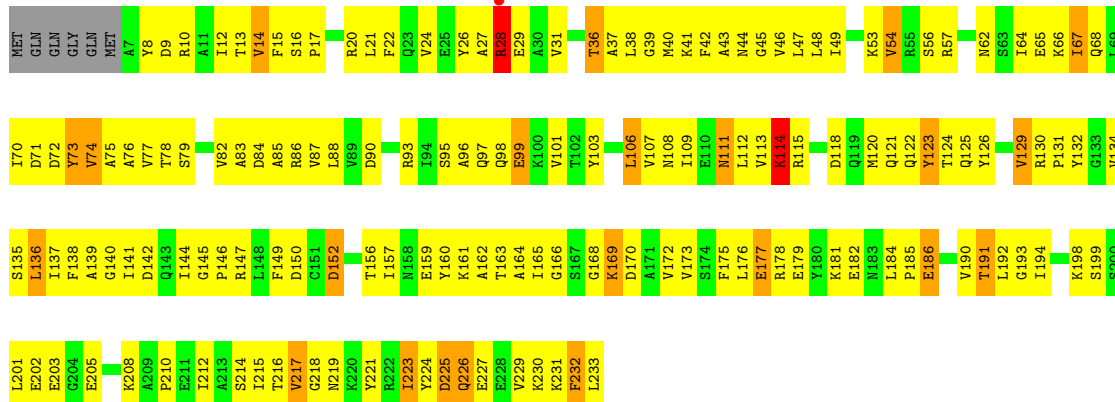


• Molecule 1: Proteasome subunit alpha



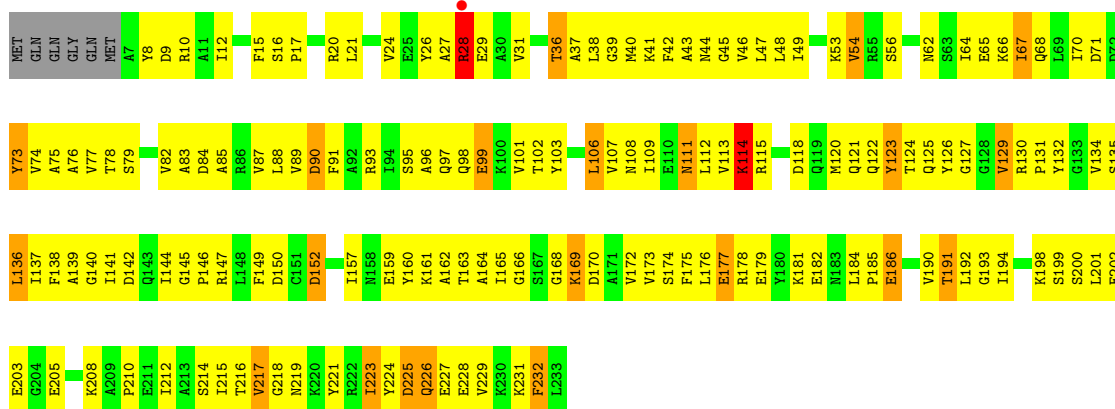
• Molecule 1: Proteasome subunit alpha

Chain F:  28% 59% 9% ..



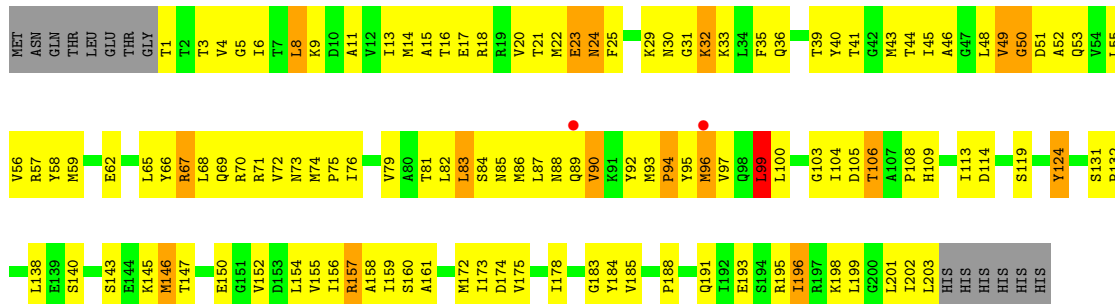
• Molecule 1: Proteasome subunit alpha

Chain G:  29% 58% 9% ..




• Molecule 2: Proteasome subunit beta

Chain H:  37% 49% 7% 6%

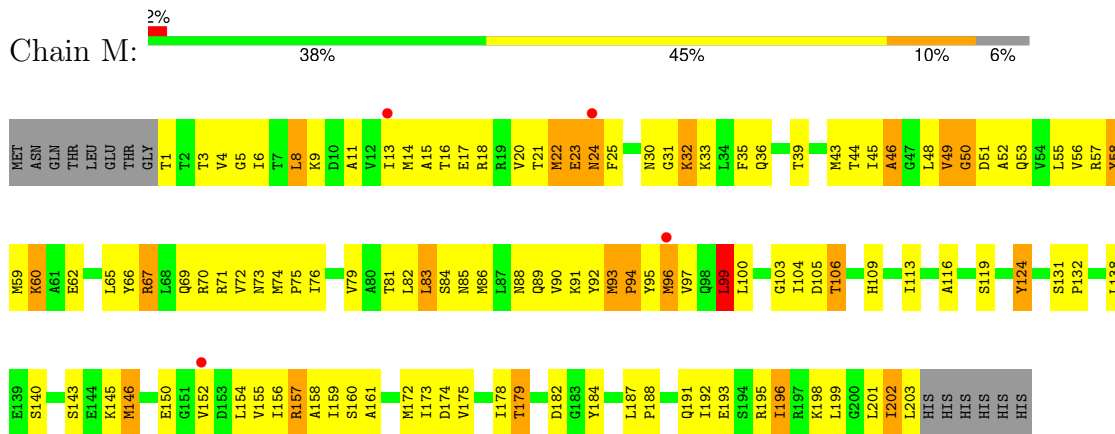


• Molecule 2: Proteasome subunit beta

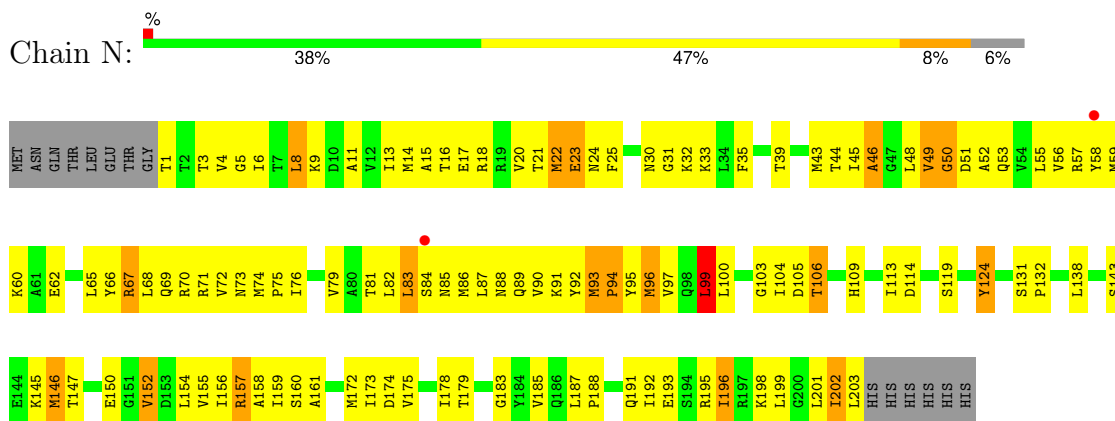
Chain I:  38% 46% 9% 6%



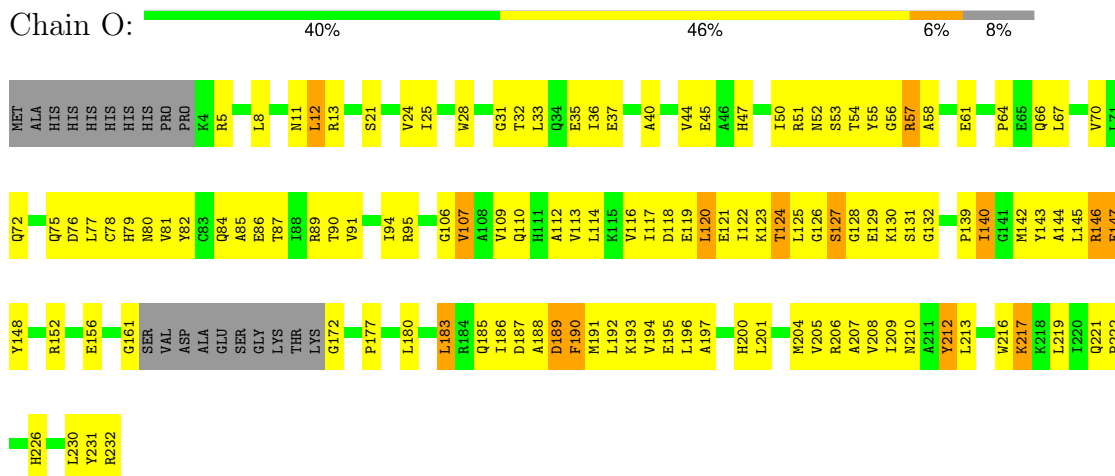
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

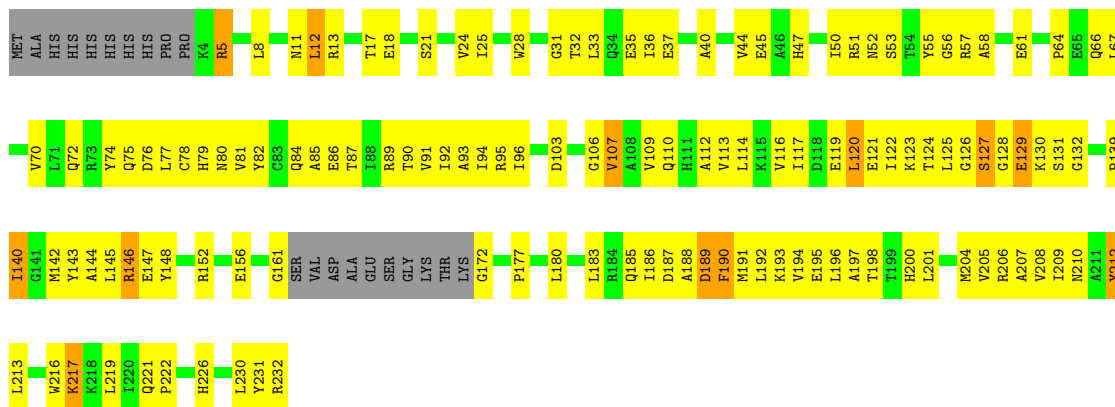


- Molecule 3: Proteasome activator PA26, Proteasome-activating nucleotidase fusion protein



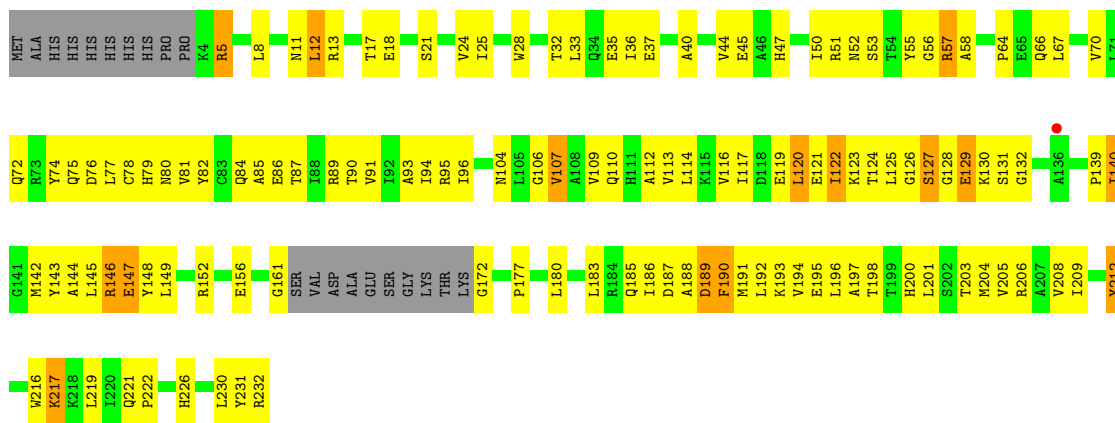
- Molecule 3: Proteasome activator PA26, Proteasome-activating nucleotidase fusion protein





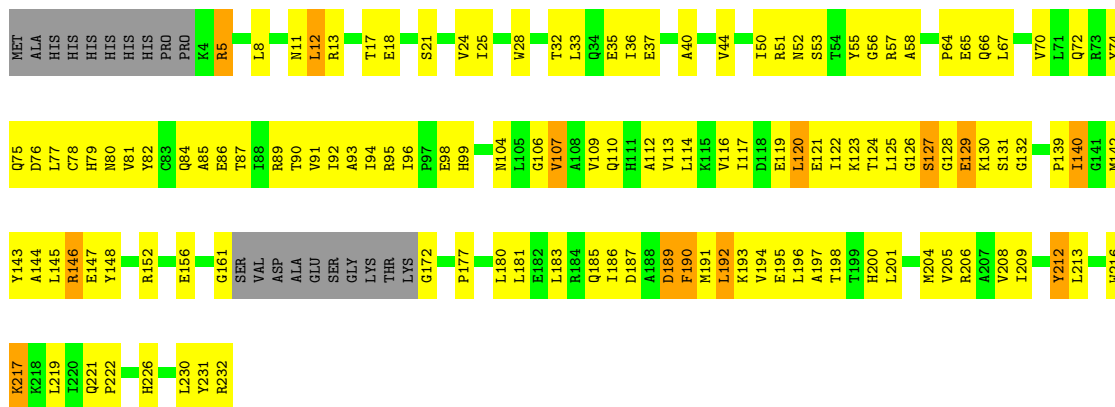
- Molecule 3: Proteasome activator PA26, Proteasome-activating nucleotidase fusion protein

Chain Q: 39% 46% 6% 8%



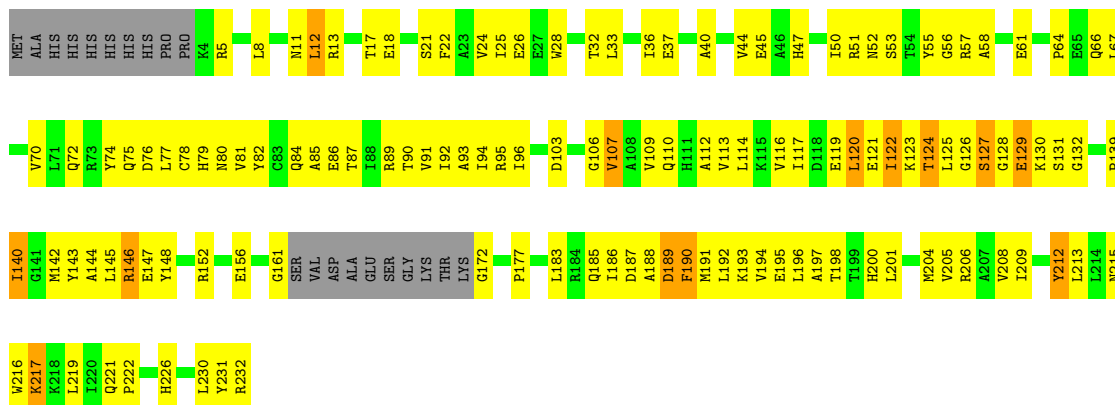
- Molecule 3: Proteasome activator PA26, Proteasome-activating nucleotidase fusion protein

Chain R: 38% 48% 5% 8%

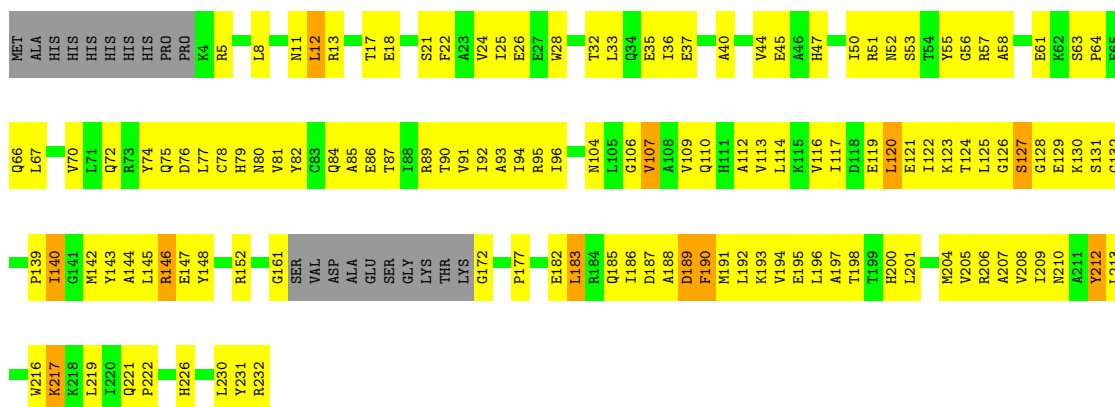


- Molecule 3: Proteasome activator PA26, Proteasome-activating nucleotidase fusion protein

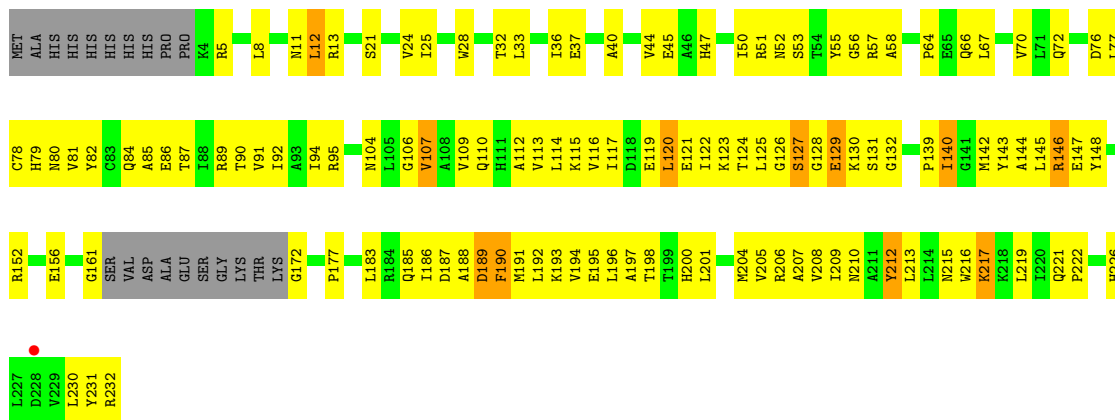
Chain S: 38% 48% 5% 8%



● Molecule 3: Proteasome activator PA26, Proteasome-activating nucleotidase fusion protein



● Molecule 3: Proteasome activator PA26, Proteasome-activating nucleotidase fusion protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.89Å 166.89Å 412.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.51 – 4.00 89.51 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (89.51-4.00) 97.4 (89.51-4.00)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 4.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.284 0.253 , 0.251	Depositor DCC
$R_{free}$ test set	2470 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.4	Xtrriage
Anisotropy	0.132	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 82.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	35133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.51	0/1793	0.99	6/2416 (0.2%)
1	B	0.51	0/1793	0.99	8/2416 (0.3%)
1	C	0.51	0/1793	0.99	8/2416 (0.3%)
1	D	0.51	0/1793	0.99	6/2416 (0.2%)
1	E	0.49	0/1793	1.00	5/2416 (0.2%)
1	F	0.49	0/1793	0.98	5/2416 (0.2%)
1	G	0.50	0/1793	0.98	6/2416 (0.2%)
2	H	0.58	0/1576	1.01	9/2129 (0.4%)
2	I	0.58	0/1576	1.01	8/2129 (0.4%)
2	J	0.55	0/1576	1.01	9/2129 (0.4%)
2	K	0.54	0/1576	1.01	7/2129 (0.3%)
2	L	0.57	0/1576	1.01	8/2129 (0.4%)
2	M	0.55	0/1576	1.00	9/2129 (0.4%)
2	N	0.57	0/1576	1.01	9/2129 (0.4%)
3	O	0.50	0/1717	0.90	2/2321 (0.1%)
3	P	0.48	0/1717	0.90	0/2321
3	Q	0.49	0/1717	0.90	0/2321
3	R	0.49	0/1717	0.90	1/2321 (0.0%)
3	S	0.49	0/1717	0.91	1/2321 (0.0%)
3	T	0.49	0/1717	0.91	4/2321 (0.2%)
3	U	0.48	0/1717	0.91	0/2321
All	All	0.52	0/35602	0.97	111/48062 (0.2%)

There are no bond length outliers.

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	161	LYS	N-CA-C	-11.15	99.92	114.31
1	G	161	LYS	N-CA-C	-11.06	100.05	114.31
1	E	161	LYS	N-CA-C	-10.92	100.22	114.31
1	D	161	LYS	N-CA-C	-10.89	100.26	114.31
1	C	161	LYS	N-CA-C	-10.83	100.34	114.31

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	1769	0	1800	189	1
1	B	1769	0	1800	199	0
1	C	1769	0	1800	196	0
1	D	1769	0	1800	207	1
1	E	1769	0	1800	208	0
1	F	1769	0	1800	197	0
1	G	1769	0	1800	194	0
2	H	1557	0	1609	137	0
2	I	1557	0	1609	139	0
2	J	1557	0	1609	125	0
2	K	1557	0	1609	128	0
2	L	1557	0	1609	129	0
2	M	1557	0	1609	135	0
2	N	1557	0	1609	134	0
3	O	1693	0	1722	141	1
3	P	1693	0	1722	150	0
3	Q	1693	0	1722	151	0
3	R	1693	0	1722	162	1
3	S	1693	0	1722	159	0
3	T	1693	0	1722	164	0
3	U	1693	0	1722	152	0
All	All	35133	0	35917	3159	2

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 44.

The worst 5 of 3159 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:N:39:THR:HB	2:N:73:ASN:HD21	1.11	1.15
2:M:39:THR:HB	2:M:73:ASN:HD21	1.08	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:39:THR:HB	2:K:73:ASN:HD21	1.10	1.13
2:I:39:THR:HB	2:I:73:ASN:HD21	1.11	1.13
2:L:39:THR:HB	2:L:73:ASN:HD21	1.12	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ARG:NH2	3:O:54:THR:O[6_566]	2.07	0.13
1:A:204:GLY:O	3:R:65:GLU:OE1[6_556]	2.19	0.01

## 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	225/233 (97%)	168 (75%)	45 (20%)	12 (5%)	1	18
1	B	225/233 (97%)	169 (75%)	44 (20%)	12 (5%)	1	18
1	C	225/233 (97%)	169 (75%)	45 (20%)	11 (5%)	1	19
1	D	225/233 (97%)	171 (76%)	44 (20%)	10 (4%)	2	20
1	E	225/233 (97%)	169 (75%)	44 (20%)	12 (5%)	1	18
1	F	225/233 (97%)	169 (75%)	45 (20%)	11 (5%)	1	19
1	G	225/233 (97%)	169 (75%)	45 (20%)	11 (5%)	1	19
2	H	201/217 (93%)	154 (77%)	38 (19%)	9 (4%)	2	20
2	I	201/217 (93%)	153 (76%)	38 (19%)	10 (5%)	1	18
2	J	201/217 (93%)	153 (76%)	36 (18%)	12 (6%)	1	16
2	K	201/217 (93%)	154 (77%)	37 (18%)	10 (5%)	1	18
2	L	201/217 (93%)	154 (77%)	38 (19%)	9 (4%)	2	20
2	M	201/217 (93%)	155 (77%)	36 (18%)	10 (5%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	201/217 (93%)	153 (76%)	38 (19%)	10 (5%)	1	18
3	O	215/239 (90%)	168 (78%)	38 (18%)	9 (4%)	2	21
3	P	215/239 (90%)	167 (78%)	38 (18%)	10 (5%)	2	19
3	Q	215/239 (90%)	168 (78%)	37 (17%)	10 (5%)	2	19
3	R	215/239 (90%)	167 (78%)	38 (18%)	10 (5%)	2	19
3	S	215/239 (90%)	166 (77%)	40 (19%)	9 (4%)	2	21
3	T	215/239 (90%)	169 (79%)	37 (17%)	9 (4%)	2	21
3	U	215/239 (90%)	169 (79%)	36 (17%)	10 (5%)	2	19
All	All	4487/4823 (93%)	3434 (76%)	837 (19%)	216 (5%)	2	19

5 of 216 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	LYS
1	A	186	GLU
1	A	217	VAL
1	B	169	LYS
1	B	186	GLU

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/193 (97%)	172 (92%)	16 (8%)	10	33
1	B	188/193 (97%)	171 (91%)	17 (9%)	9	31
1	C	188/193 (97%)	170 (90%)	18 (10%)	8	28
1	D	188/193 (97%)	169 (90%)	19 (10%)	7	26
1	E	188/193 (97%)	172 (92%)	16 (8%)	10	33
1	F	188/193 (97%)	170 (90%)	18 (10%)	8	28
1	G	188/193 (97%)	171 (91%)	17 (9%)	9	31
2	H	170/183 (93%)	160 (94%)	10 (6%)	18	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	170/183 (93%)	159 (94%)	11 (6%)	15	40
2	J	170/183 (93%)	160 (94%)	10 (6%)	18	42
2	K	170/183 (93%)	160 (94%)	10 (6%)	18	42
2	L	170/183 (93%)	160 (94%)	10 (6%)	18	42
2	M	170/183 (93%)	158 (93%)	12 (7%)	13	38
2	N	170/183 (93%)	160 (94%)	10 (6%)	18	42
3	O	179/196 (91%)	171 (96%)	8 (4%)	24	47
3	P	179/196 (91%)	171 (96%)	8 (4%)	24	47
3	Q	179/196 (91%)	170 (95%)	9 (5%)	22	45
3	R	179/196 (91%)	171 (96%)	8 (4%)	24	47
3	S	179/196 (91%)	170 (95%)	9 (5%)	22	45
3	T	179/196 (91%)	171 (96%)	8 (4%)	24	47
3	U	179/196 (91%)	171 (96%)	8 (4%)	24	47
All	All	3759/4004 (94%)	3507 (93%)	252 (7%)	15	39

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	177	GLU
3	R	120	LEU
2	J	20	VAL
3	R	11	ASN
3	T	11	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	73	ASN
3	O	72	GLN
2	L	141	GLN
2	N	30	ASN
3	P	72	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	227/233 (97%)	-0.13	2 (0%) 81 64	26, 89, 125, 148	2 (0%)
1	B	227/233 (97%)	-0.11	2 (0%) 81 64	26, 88, 123, 148	2 (0%)
1	C	227/233 (97%)	-0.13	2 (0%) 81 64	26, 88, 124, 146	2 (0%)
1	D	227/233 (97%)	-0.09	2 (0%) 81 64	25, 87, 125, 147	2 (0%)
1	E	227/233 (97%)	-0.21	2 (0%) 81 64	25, 88, 123, 147	2 (0%)
1	F	227/233 (97%)	-0.18	1 (0%) 88 75	26, 87, 124, 146	1 (0%)
1	G	227/233 (97%)	-0.23	1 (0%) 88 75	25, 88, 124, 146	1 (0%)
2	H	203/217 (93%)	-0.10	2 (0%) 79 61	24, 87, 111, 172	4 (1%)
2	I	203/217 (93%)	-0.11	2 (0%) 79 61	24, 87, 112, 171	3 (1%)
2	J	203/217 (93%)	-0.12	1 (0%) 87 73	24, 87, 111, 172	4 (1%)
2	K	203/217 (93%)	-0.17	1 (0%) 87 73	25, 86, 111, 172	4 (1%)
2	L	203/217 (93%)	-0.16	1 (0%) 87 73	24, 87, 112, 171	4 (1%)
2	M	203/217 (93%)	-0.13	4 (1%) 65 48	24, 87, 111, 172	3 (1%)
2	N	203/217 (93%)	-0.09	2 (0%) 79 61	24, 87, 112, 172	4 (1%)
3	O	219/239 (91%)	-0.14	0 100 100	66, 97, 136, 174	0
3	P	219/239 (91%)	-0.16	0 100 100	65, 97, 135, 173	0
3	Q	219/239 (91%)	-0.15	1 (0%) 87 73	65, 97, 135, 174	0
3	R	219/239 (91%)	-0.15	0 100 100	66, 97, 136, 174	0
3	S	219/239 (91%)	-0.16	0 100 100	65, 98, 137, 175	0
3	T	219/239 (91%)	-0.05	0 100 100	66, 98, 137, 174	0
3	U	219/239 (91%)	-0.19	1 (0%) 87 73	64, 98, 137, 173	0
All	All	4543/4823 (94%)	-0.14	27 (0%) 85 71	24, 91, 128, 175	38 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	77	VAL	4.2
1	A	77	VAL	3.7
2	K	89	GLN	3.3
1	C	77	VAL	3.2
2	M	152	VAL	3.0

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.