



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 07:02 AM EDT

PDB ID : 6Z46
Title : Structure of the *S. acidocaldarius* 20S proteasome (Saci0613/Saci0662)
Authors : Robinson, N.P.; Bray, S.M.
Deposited on : 2020-05-22
Resolution : 3.70 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

<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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

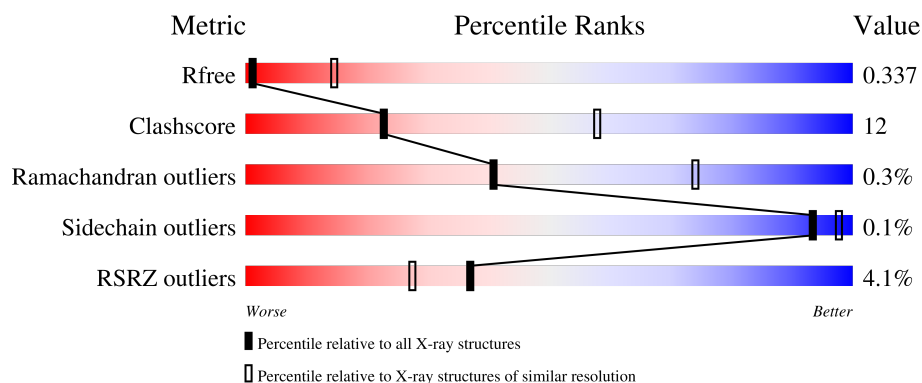
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	242	<div> <div>5%</div> <div>62% 28% 10%</div> </div>
1	B	242	<div> <div>68% 24% 8%</div> </div>
1	C	242	<div> <div>5%</div> <div>65% 24% 10%</div> </div>
1	D	242	<div> <div>5%</div> <div>62% 25% 13%</div> </div>
1	E	242	<div> <div>6%</div> <div>58% 32% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	242	
1	G	242	
1	O	242	
1	P	242	
1	Q	242	
1	R	242	
1	S	242	
1	T	242	
1	U	242	
2	H	198	
2	I	198	
2	J	198	
2	K	198	
2	L	198	
2	M	198	
2	N	198	
2	V	198	
2	W	198	
2	X	198	
2	Y	198	
2	Z	198	
2	a	198	
2	b	198	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41436 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	218	Total	C	N	O	S	0	0	0
			1687	1083	276	322	6			
1	B	223	Total	C	N	O	S	0	0	0
			1740	1116	284	335	5			
1	C	218	Total	C	N	O	S	0	0	0
			1699	1090	277	327	5			
1	D	211	Total	C	N	O	S	0	0	0
			1642	1053	270	315	4			
1	E	219	Total	C	N	O	S	0	0	0
			1706	1093	279	329	5			
1	F	219	Total	C	N	O	S	0	0	0
			1706	1093	279	329	5			
1	G	220	Total	C	N	O	S	0	0	0
			1714	1099	280	330	5			
1	O	213	Total	C	N	O	S	0	0	0
			1656	1060	270	321	5			
1	P	203	Total	C	N	O	S	0	0	0
			1580	1012	256	307	5			
1	Q	201	Total	C	N	O	S	0	0	0
			1560	1001	255	300	4			
1	R	161	Total	C	N	O	S	0	0	0
			1250	808	203	235	4			
1	S	189	Total	C	N	O	S	0	0	0
			1454	934	239	276	5			
1	T	202	Total	C	N	O	S	0	0	0
			1562	1002	258	298	4			
1	U	205	Total	C	N	O	S	0	0	0
			1589	1022	259	303	5			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	183	Total	C	N	O	S	0	1	0
			1405	905	229	267	4			
2	I	182	Total	C	N	O	S	0	0	0
			1381	882	232	263	4			
2	J	180	Total	C	N	O	S	0	0	0
			1369	876	230	259	4			
2	K	179	Total	C	N	O	S	0	0	0
			1357	868	227	258	4			
2	L	181	Total	C	N	O	S	0	0	0
			1373	876	231	262	4			
2	M	175	Total	C	N	O	S	0	0	0
			1324	846	221	253	4			
2	N	183	Total	C	N	O	S	0	0	0
			1393	891	233	265	4			
2	V	184	Total	C	N	O	S	0	0	0
			1402	896	234	268	4			
2	W	163	Total	C	N	O	S	0	0	0
			1233	787	205	237	4			
2	X	174	Total	C	N	O	S	0	0	0
			1311	840	217	250	4			
2	Y	177	Total	C	N	O	S	0	0	0
			1345	863	223	255	4			
2	Z	178	Total	C	N	O	S	0	0	0
			1347	861	227	255	4			
2	a	174	Total	C	N	O	S	0	0	0
			1319	846	219	250	4			
2	b	176	Total	C	N	O	S	0	0	0
			1332	852	222	254	4			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	initiating methionine	UNP A0A0U3GVH3
H	191	LEU	-	expression tag	UNP A0A0U3GVH3
H	192	GLU	-	expression tag	UNP A0A0U3GVH3
H	193	HIS	-	expression tag	UNP A0A0U3GVH3
H	194	HIS	-	expression tag	UNP A0A0U3GVH3
H	195	HIS	-	expression tag	UNP A0A0U3GVH3
H	196	HIS	-	expression tag	UNP A0A0U3GVH3
H	197	HIS	-	expression tag	UNP A0A0U3GVH3
H	198	HIS	-	expression tag	UNP A0A0U3GVH3
I	1	MET	-	initiating methionine	UNP A0A0U3GVH3
I	191	LEU	-	expression tag	UNP A0A0U3GVH3
I	192	GLU	-	expression tag	UNP A0A0U3GVH3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	193	HIS	-	expression tag	UNP A0A0U3GVH3
I	194	HIS	-	expression tag	UNP A0A0U3GVH3
I	195	HIS	-	expression tag	UNP A0A0U3GVH3
I	196	HIS	-	expression tag	UNP A0A0U3GVH3
I	197	HIS	-	expression tag	UNP A0A0U3GVH3
I	198	HIS	-	expression tag	UNP A0A0U3GVH3
J	1	MET	-	initiating methionine	UNP A0A0U3GVH3
J	191	LEU	-	expression tag	UNP A0A0U3GVH3
J	192	GLU	-	expression tag	UNP A0A0U3GVH3
J	193	HIS	-	expression tag	UNP A0A0U3GVH3
J	194	HIS	-	expression tag	UNP A0A0U3GVH3
J	195	HIS	-	expression tag	UNP A0A0U3GVH3
J	196	HIS	-	expression tag	UNP A0A0U3GVH3
J	197	HIS	-	expression tag	UNP A0A0U3GVH3
J	198	HIS	-	expression tag	UNP A0A0U3GVH3
K	1	MET	-	initiating methionine	UNP A0A0U3GVH3
K	191	LEU	-	expression tag	UNP A0A0U3GVH3
K	192	GLU	-	expression tag	UNP A0A0U3GVH3
K	193	HIS	-	expression tag	UNP A0A0U3GVH3
K	194	HIS	-	expression tag	UNP A0A0U3GVH3
K	195	HIS	-	expression tag	UNP A0A0U3GVH3
K	196	HIS	-	expression tag	UNP A0A0U3GVH3
K	197	HIS	-	expression tag	UNP A0A0U3GVH3
K	198	HIS	-	expression tag	UNP A0A0U3GVH3
L	1	MET	-	initiating methionine	UNP A0A0U3GVH3
L	191	LEU	-	expression tag	UNP A0A0U3GVH3
L	192	GLU	-	expression tag	UNP A0A0U3GVH3
L	193	HIS	-	expression tag	UNP A0A0U3GVH3
L	194	HIS	-	expression tag	UNP A0A0U3GVH3
L	195	HIS	-	expression tag	UNP A0A0U3GVH3
L	196	HIS	-	expression tag	UNP A0A0U3GVH3
L	197	HIS	-	expression tag	UNP A0A0U3GVH3
L	198	HIS	-	expression tag	UNP A0A0U3GVH3
M	1	MET	-	initiating methionine	UNP A0A0U3GVH3
M	191	LEU	-	expression tag	UNP A0A0U3GVH3
M	192	GLU	-	expression tag	UNP A0A0U3GVH3
M	193	HIS	-	expression tag	UNP A0A0U3GVH3
M	194	HIS	-	expression tag	UNP A0A0U3GVH3
M	195	HIS	-	expression tag	UNP A0A0U3GVH3
M	196	HIS	-	expression tag	UNP A0A0U3GVH3
M	197	HIS	-	expression tag	UNP A0A0U3GVH3
M	198	HIS	-	expression tag	UNP A0A0U3GVH3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	1	MET	-	initiating methionine	UNP A0A0U3GVH3
N	191	LEU	-	expression tag	UNP A0A0U3GVH3
N	192	GLU	-	expression tag	UNP A0A0U3GVH3
N	193	HIS	-	expression tag	UNP A0A0U3GVH3
N	194	HIS	-	expression tag	UNP A0A0U3GVH3
N	195	HIS	-	expression tag	UNP A0A0U3GVH3
N	196	HIS	-	expression tag	UNP A0A0U3GVH3
N	197	HIS	-	expression tag	UNP A0A0U3GVH3
N	198	HIS	-	expression tag	UNP A0A0U3GVH3
V	1	MET	-	initiating methionine	UNP A0A0U3GVH3
V	191	LEU	-	expression tag	UNP A0A0U3GVH3
V	192	GLU	-	expression tag	UNP A0A0U3GVH3
V	193	HIS	-	expression tag	UNP A0A0U3GVH3
V	194	HIS	-	expression tag	UNP A0A0U3GVH3
V	195	HIS	-	expression tag	UNP A0A0U3GVH3
V	196	HIS	-	expression tag	UNP A0A0U3GVH3
V	197	HIS	-	expression tag	UNP A0A0U3GVH3
V	198	HIS	-	expression tag	UNP A0A0U3GVH3
W	1	MET	-	initiating methionine	UNP A0A0U3GVH3
W	191	LEU	-	expression tag	UNP A0A0U3GVH3
W	192	GLU	-	expression tag	UNP A0A0U3GVH3
W	193	HIS	-	expression tag	UNP A0A0U3GVH3
W	194	HIS	-	expression tag	UNP A0A0U3GVH3
W	195	HIS	-	expression tag	UNP A0A0U3GVH3
W	196	HIS	-	expression tag	UNP A0A0U3GVH3
W	197	HIS	-	expression tag	UNP A0A0U3GVH3
W	198	HIS	-	expression tag	UNP A0A0U3GVH3
X	1	MET	-	initiating methionine	UNP A0A0U3GVH3
X	191	LEU	-	expression tag	UNP A0A0U3GVH3
X	192	GLU	-	expression tag	UNP A0A0U3GVH3
X	193	HIS	-	expression tag	UNP A0A0U3GVH3
X	194	HIS	-	expression tag	UNP A0A0U3GVH3
X	195	HIS	-	expression tag	UNP A0A0U3GVH3
X	196	HIS	-	expression tag	UNP A0A0U3GVH3
X	197	HIS	-	expression tag	UNP A0A0U3GVH3
X	198	HIS	-	expression tag	UNP A0A0U3GVH3
Y	1	MET	-	initiating methionine	UNP A0A0U3GVH3
Y	191	LEU	-	expression tag	UNP A0A0U3GVH3
Y	192	GLU	-	expression tag	UNP A0A0U3GVH3
Y	193	HIS	-	expression tag	UNP A0A0U3GVH3
Y	194	HIS	-	expression tag	UNP A0A0U3GVH3
Y	195	HIS	-	expression tag	UNP A0A0U3GVH3

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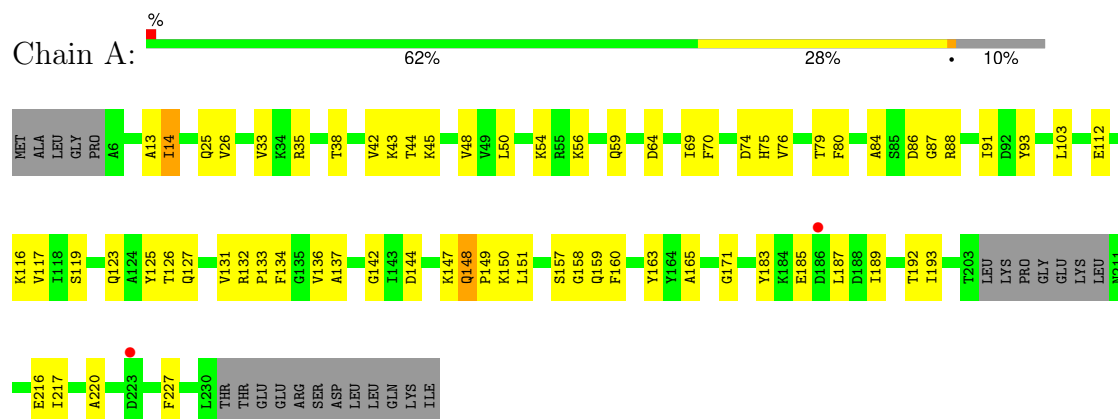
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Chain	Residue	Modelled	Actual	Comment	Reference
Y	196	HIS	-	expression tag	UNP A0A0U3GVH3
Y	197	HIS	-	expression tag	UNP A0A0U3GVH3
Y	198	HIS	-	expression tag	UNP A0A0U3GVH3
Z	1	MET	-	initiating methionine	UNP A0A0U3GVH3
Z	191	LEU	-	expression tag	UNP A0A0U3GVH3
Z	192	GLU	-	expression tag	UNP A0A0U3GVH3
Z	193	HIS	-	expression tag	UNP A0A0U3GVH3
Z	194	HIS	-	expression tag	UNP A0A0U3GVH3
Z	195	HIS	-	expression tag	UNP A0A0U3GVH3
Z	196	HIS	-	expression tag	UNP A0A0U3GVH3
Z	197	HIS	-	expression tag	UNP A0A0U3GVH3
Z	198	HIS	-	expression tag	UNP A0A0U3GVH3
a	1	MET	-	initiating methionine	UNP A0A0U3GVH3
a	191	LEU	-	expression tag	UNP A0A0U3GVH3
a	192	GLU	-	expression tag	UNP A0A0U3GVH3
a	193	HIS	-	expression tag	UNP A0A0U3GVH3
a	194	HIS	-	expression tag	UNP A0A0U3GVH3
a	195	HIS	-	expression tag	UNP A0A0U3GVH3
a	196	HIS	-	expression tag	UNP A0A0U3GVH3
a	197	HIS	-	expression tag	UNP A0A0U3GVH3
a	198	HIS	-	expression tag	UNP A0A0U3GVH3
b	1	MET	-	initiating methionine	UNP A0A0U3GVH3
b	191	LEU	-	expression tag	UNP A0A0U3GVH3
b	192	GLU	-	expression tag	UNP A0A0U3GVH3
b	193	HIS	-	expression tag	UNP A0A0U3GVH3
b	194	HIS	-	expression tag	UNP A0A0U3GVH3
b	195	HIS	-	expression tag	UNP A0A0U3GVH3
b	196	HIS	-	expression tag	UNP A0A0U3GVH3
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b	198	HIS	-	expression tag	UNP A0A0U3GVH3

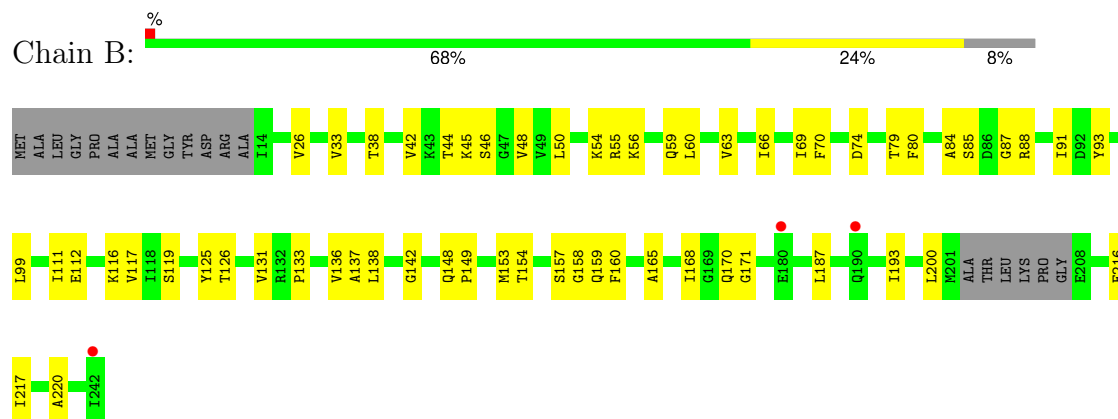
3 Residue-property plots

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.

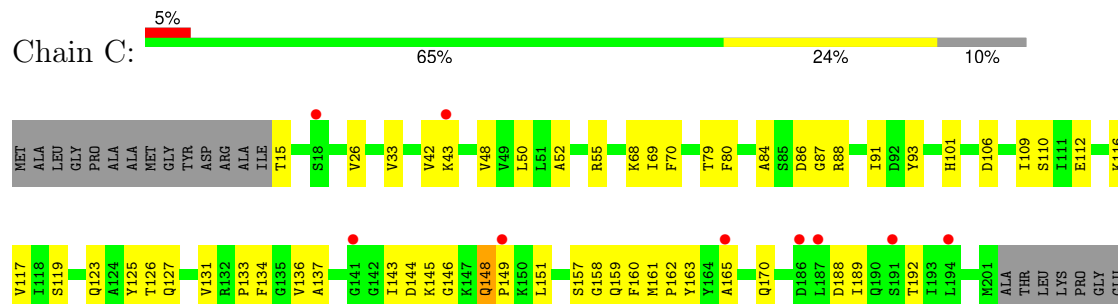
• Molecule 1: Proteasome subunit alpha



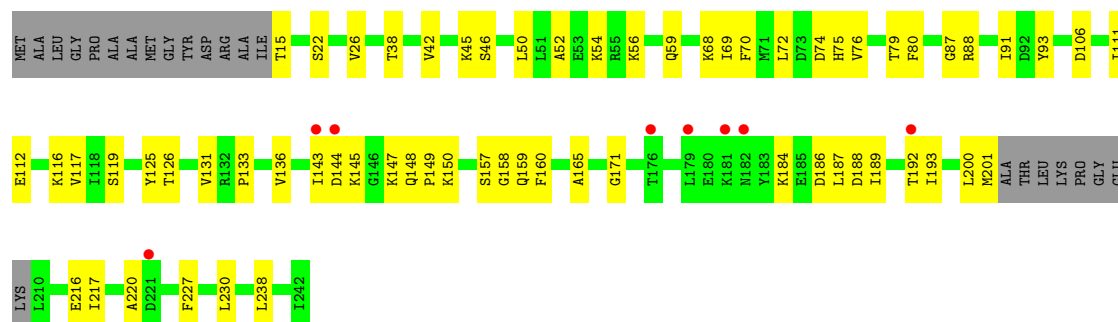
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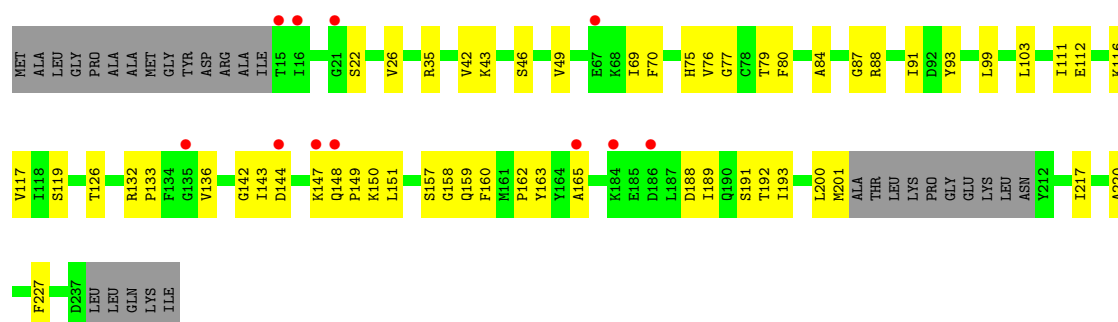
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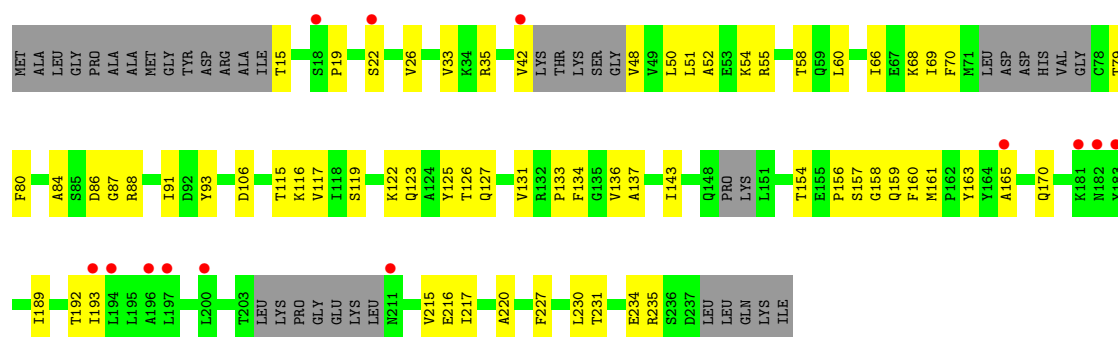




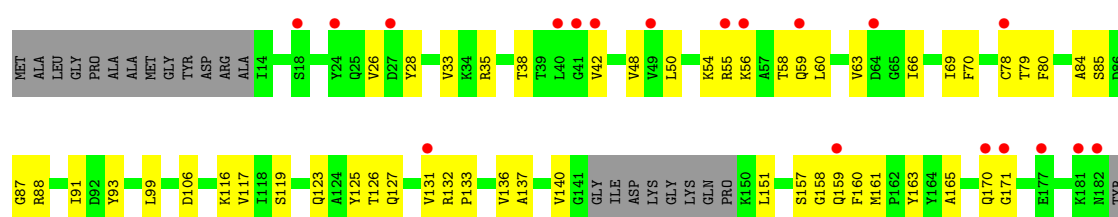
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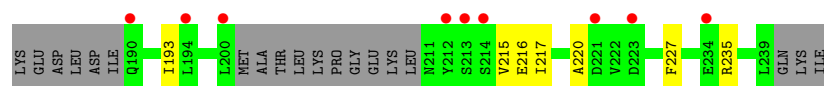


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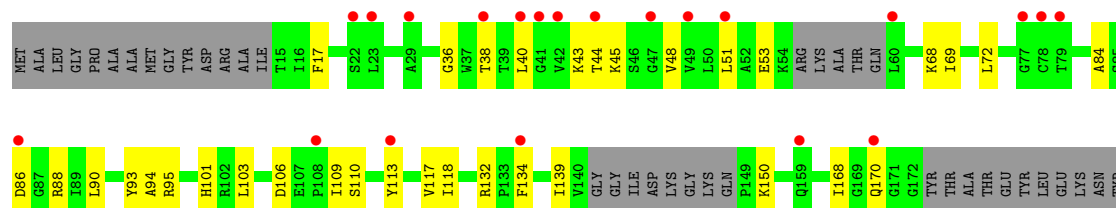


• Molecule 1: Proteasome subunit alpha

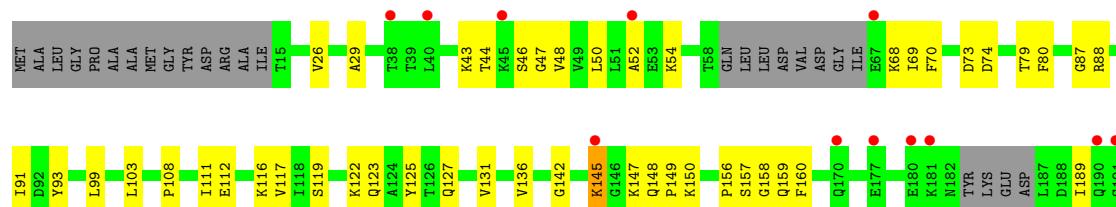




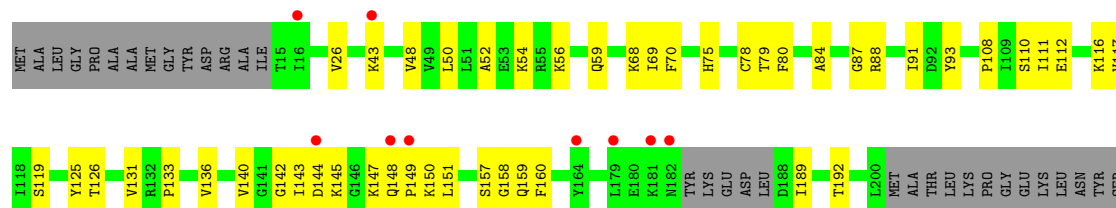
• Molecule 1: Proteasome subunit alpha



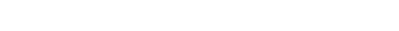
• Molecule 1: Proteasome subunit alpha

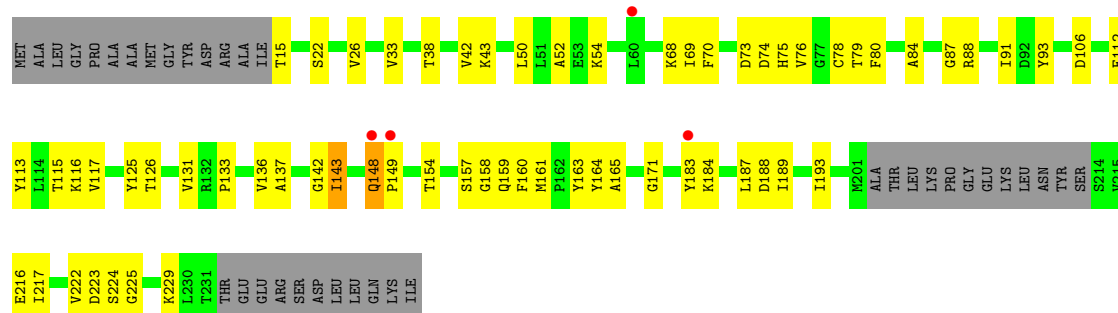


• Molecule 1: Proteasome subunit alpha

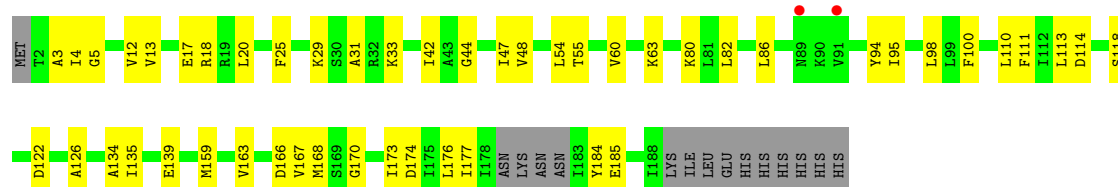


• Molecule 1: Proteasome subunit alpha

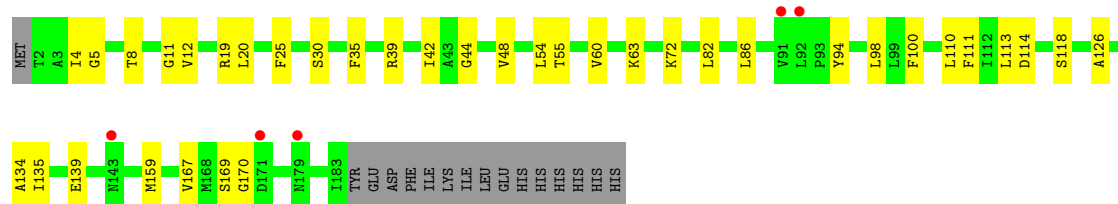




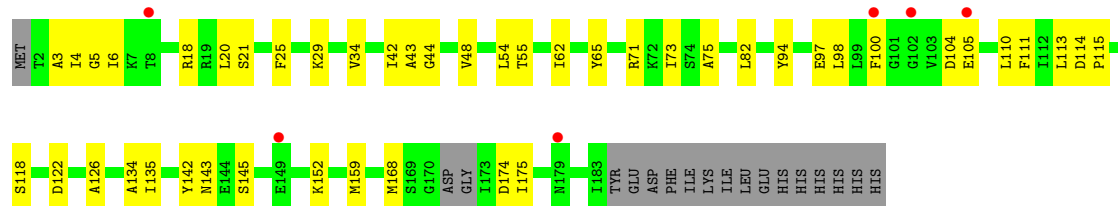
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

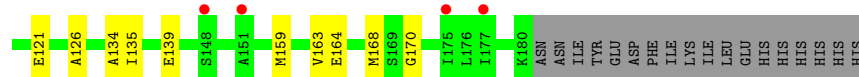


• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

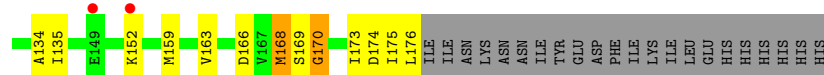




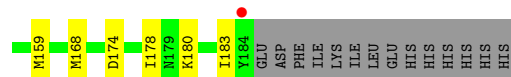
• Molecule 2: Proteasome subunit beta



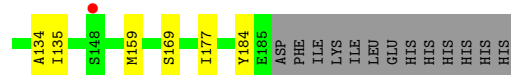
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

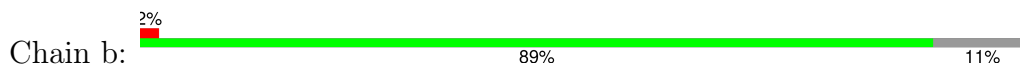


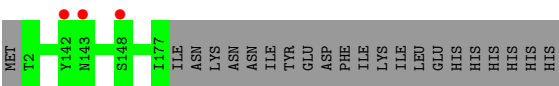
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.29Å 193.65Å 323.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.19 – 3.70 48.29 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.19-3.70) 99.3 (48.29-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.287 , 0.334 0.289 , 0.337	Depositor DCC
R_{free} test set	3677 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	41436	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	A	0.25	0/1717	0.47	0/2320
1	B	0.25	0/1769	0.47	0/2387
1	C	0.25	0/1728	0.45	0/2333
1	D	0.25	0/1670	0.45	0/2254
1	E	0.24	0/1735	0.44	0/2342
1	F	0.26	0/1735	0.48	0/2342
1	G	0.24	0/1743	0.46	0/2353
1	O	0.25	0/1685	0.45	0/2275
1	P	0.24	0/1604	0.42	0/2163
1	Q	0.24	0/1585	0.44	0/2140
1	R	0.24	0/1272	0.45	0/1713
1	S	0.24	0/1478	0.44	0/1996
1	T	0.24	0/1587	0.44	0/2142
1	U	0.25	0/1617	0.45	0/2184
2	H	0.24	0/1425	0.42	0/1917
2	I	0.23	0/1396	0.40	0/1878
2	J	0.24	0/1383	0.42	0/1859
2	K	0.24	0/1372	0.44	0/1845
2	L	0.24	0/1388	0.42	0/1867
2	M	0.27	0/1339	0.43	0/1801
2	N	0.24	0/1409	0.42	0/1896
2	V	0.23	0/1418	0.41	0/1908
2	W	0.23	0/1246	0.41	0/1676
2	X	0.24	0/1324	0.42	0/1780
2	Y	0.24	0/1359	0.42	0/1827
2	Z	0.24	0/1360	0.44	0/1827
2	a	0.24	0/1333	0.43	0/1793
2	b	0.24	0/1347	0.45	0/1812
All	All	0.24	0/42024	0.44	0/56630

There are no bond length outliers.

There are no bond angle outliers.

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	1687	0	1699	59	0
1	B	1740	0	1758	46	0
1	C	1699	0	1715	51	0
1	D	1642	0	1657	51	0
1	E	1706	0	1717	62	0
1	F	1706	0	1717	49	0
1	G	1714	0	1728	51	0
1	O	1656	0	1657	52	0
1	P	1580	0	1573	50	0
1	Q	1560	0	1565	44	0
1	R	1250	0	1252	27	0
1	S	1454	0	1469	38	0
1	T	1562	0	1577	44	0
1	U	1589	0	1606	52	0
2	H	1405	0	1458	35	0
2	I	1381	0	1442	27	0
2	J	1369	0	1434	27	0
2	K	1357	0	1419	30	0
2	L	1373	0	1431	38	0
2	M	1324	0	1378	33	0
2	N	1393	0	1451	26	0
2	V	1402	0	1457	26	0
2	W	1233	0	1281	21	0
2	X	1311	0	1372	30	0
2	Y	1345	0	1398	28	0
2	Z	1347	0	1415	40	0
2	a	1319	0	1379	0	0
2	b	1332	0	1389	0	0
All	All	41436	0	42394	911	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 12.

The worst 5 of 911 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:A:43:LYS:HD2	1:A:151:LEU:HB2	1.50	0.91
2:M:19:ARG:HD3	2:M:169:SER:HA	1.55	0.87
2:K:163:VAL:HG22	2:K:170:GLY:HA2	1.57	0.85
1:Q:54:LYS:HD2	1:Q:216:GLU:HG3	1.58	0.84
1:B:44:THR:HB	1:B:187:LEU:HD12	1.60	0.84

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	214/242 (88%)	196 (92%)	15 (7%)	3 (1%)	11	45
1	B	219/242 (90%)	209 (95%)	10 (5%)	0	100	100
1	C	214/242 (88%)	205 (96%)	8 (4%)	1 (0%)	29	66
1	D	207/242 (86%)	199 (96%)	6 (3%)	2 (1%)	15	51
1	E	215/242 (89%)	203 (94%)	11 (5%)	1 (0%)	29	66
1	F	215/242 (89%)	204 (95%)	11 (5%)	0	100	100
1	G	216/242 (89%)	205 (95%)	10 (5%)	1 (0%)	29	66
1	O	209/242 (86%)	201 (96%)	7 (3%)	1 (0%)	29	66
1	P	193/242 (80%)	184 (95%)	9 (5%)	0	100	100
1	Q	193/242 (80%)	186 (96%)	7 (4%)	0	100	100
1	R	151/242 (62%)	144 (95%)	7 (5%)	0	100	100
1	S	181/242 (75%)	170 (94%)	10 (6%)	1 (1%)	25	62
1	T	194/242 (80%)	188 (97%)	6 (3%)	0	100	100
1	U	201/242 (83%)	194 (96%)	5 (2%)	2 (1%)	15	51
2	H	180/198 (91%)	171 (95%)	8 (4%)	1 (1%)	25	62
2	I	180/198 (91%)	171 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	176/198 (89%)	166 (94%)	10 (6%)	0	100	100
2	K	177/198 (89%)	164 (93%)	13 (7%)	0	100	100
2	L	179/198 (90%)	169 (94%)	9 (5%)	1 (1%)	25	62
2	M	173/198 (87%)	162 (94%)	9 (5%)	2 (1%)	13	48
2	N	181/198 (91%)	170 (94%)	11 (6%)	0	100	100
2	V	182/198 (92%)	173 (95%)	9 (5%)	0	100	100
2	W	159/198 (80%)	153 (96%)	6 (4%)	0	100	100
2	X	170/198 (86%)	153 (90%)	17 (10%)	0	100	100
2	Y	171/198 (86%)	159 (93%)	10 (6%)	2 (1%)	13	48
2	Z	174/198 (88%)	161 (92%)	13 (8%)	0	100	100
2	a	170/198 (86%)	163 (96%)	7 (4%)	0	100	100
2	b	174/198 (88%)	166 (95%)	8 (5%)	0	100	100
All	All	5268/6160 (86%)	4989 (95%)	261 (5%)	18 (0%)	41	74

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	C	148	GLN
1	E	181	LYS
2	L	180	LYS
2	M	168	MET

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	177/198 (89%)	177 (100%)	0	100	100
1	B	187/198 (94%)	186 (100%)	1 (0%)	88	94
1	C	182/198 (92%)	182 (100%)	0	100	100
1	D	175/198 (88%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	183/198 (92%)	183 (100%)	0	100	100
1	F	183/198 (92%)	180 (98%)	3 (2%)	62	80
1	G	184/198 (93%)	184 (100%)	0	100	100
1	O	177/198 (89%)	177 (100%)	0	100	100
1	P	168/198 (85%)	168 (100%)	0	100	100
1	Q	167/198 (84%)	167 (100%)	0	100	100
1	R	134/198 (68%)	134 (100%)	0	100	100
1	S	153/198 (77%)	153 (100%)	0	100	100
1	T	166/198 (84%)	166 (100%)	0	100	100
1	U	169/198 (85%)	169 (100%)	0	100	100
2	H	148/162 (91%)	148 (100%)	0	100	100
2	I	146/162 (90%)	146 (100%)	0	100	100
2	J	145/162 (90%)	145 (100%)	0	100	100
2	K	143/162 (88%)	143 (100%)	0	100	100
2	L	145/162 (90%)	145 (100%)	0	100	100
2	M	139/162 (86%)	139 (100%)	0	100	100
2	N	147/162 (91%)	147 (100%)	0	100	100
2	V	148/162 (91%)	148 (100%)	0	100	100
2	W	130/162 (80%)	130 (100%)	0	100	100
2	X	138/162 (85%)	138 (100%)	0	100	100
2	Y	141/162 (87%)	141 (100%)	0	100	100
2	Z	143/162 (88%)	143 (100%)	0	100	100
2	a	139/162 (86%)	139 (100%)	0	100	100
2	b	140/162 (86%)	140 (100%)	0	100	100
All	All	4397/5040 (87%)	4393 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	200	LEU
1	F	145	LYS
1	F	148	GLN
1	F	150	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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, 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	218/242 (90%)	0.19	2 (0%) 84 76	37, 65, 100, 118	0
1	B	223/242 (92%)	0.08	3 (1%) 77 67	34, 66, 102, 127	0
1	C	218/242 (90%)	0.36	12 (5%) 25 18	38, 78, 110, 128	0
1	D	211/242 (87%)	0.46	11 (5%) 27 20	46, 80, 110, 130	0
1	E	219/242 (90%)	0.43	14 (6%) 19 13	47, 81, 115, 140	0
1	F	219/242 (90%)	0.32	7 (3%) 47 35	42, 75, 104, 127	0
1	G	220/242 (90%)	0.27	8 (3%) 42 32	40, 71, 108, 134	0
1	O	213/242 (88%)	0.36	11 (5%) 27 20	55, 80, 110, 145	0
1	P	203/242 (83%)	0.47	13 (6%) 19 13	55, 95, 130, 139	0
1	Q	201/242 (83%)	0.68	28 (13%) 2 3	54, 100, 129, 159	0
1	R	161/242 (66%)	0.78	23 (14%) 2 2	60, 94, 124, 145	0
1	S	189/242 (78%)	0.47	14 (7%) 14 10	50, 84, 114, 135	0
1	T	202/242 (83%)	0.40	10 (4%) 28 21	40, 71, 100, 120	0
1	U	205/242 (84%)	0.16	4 (1%) 65 53	42, 66, 98, 118	0
2	H	183/198 (92%)	0.10	2 (1%) 80 71	43, 65, 101, 161	0
2	I	182/198 (91%)	0.18	5 (2%) 54 42	47, 70, 97, 111	0
2	J	180/198 (90%)	0.28	6 (3%) 46 35	43, 73, 98, 129	0
2	K	179/198 (90%)	0.30	7 (3%) 39 28	45, 71, 99, 112	0
2	L	181/198 (91%)	0.06	4 (2%) 62 50	41, 66, 94, 116	0
2	M	175/198 (88%)	0.07	3 (1%) 70 59	41, 67, 96, 133	0
2	N	183/198 (92%)	0.07	3 (1%) 72 61	42, 66, 98, 111	0
2	V	184/198 (92%)	0.13	2 (1%) 80 71	45, 69, 97, 111	0
2	W	163/198 (82%)	0.28	2 (1%) 79 69	49, 73, 98, 117	0
2	X	174/198 (87%)	0.37	9 (5%) 27 20	54, 75, 112, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
2	Y	177/198 (89%)	0.38	7 (3%)	38 28	47, 76, 111, 135	0
2	Z	178/198 (89%)	0.30	6 (3%)	45 34	50, 72, 102, 118	0
2	a	174/198 (87%)	0.01	1 (0%)	89 83	42, 65, 93, 106	0
2	b	176/198 (88%)	0.04	3 (1%)	70 59	41, 63, 92, 114	0
All	All	5391/6160 (87%)	0.29	220 (4%)	37 27	34, 74, 111, 161	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	144	ASP	6.4
2	Z	102	GLY	4.9
1	T	149	PRO	4.7
1	R	51	LEU	4.7
1	D	240	GLN	4.6

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.