



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:48 PM UTC

PDB ID : 3UNE / pdb\_00003une  
Title : Mouse constitutive 20S proteasome  
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.  
Deposited on : 2011-11-15  
Resolution : 3.20 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (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

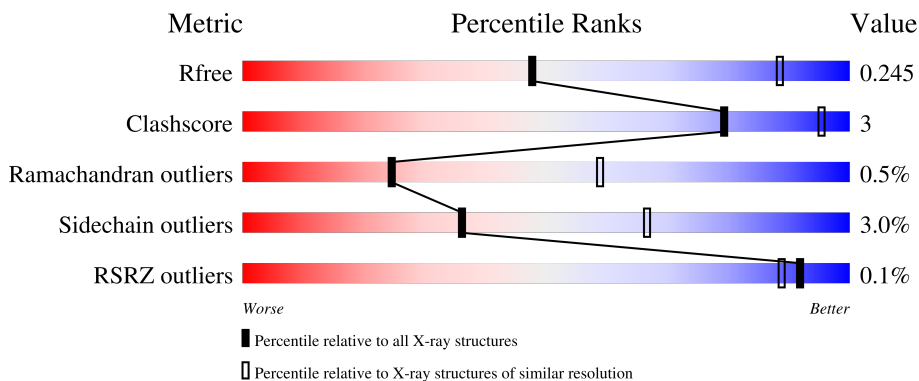
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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

























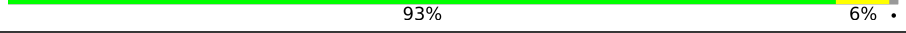


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	234	 81% 18% .
1	O	234	 83% 16%
1	c	234	 85% 13% .
1	q	234	 84% 15%
2	B	261	 89% 7% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	P	261	 89% 7% 5%
2	d	261	 86% 8% 5%
2	r	261	 89% 7% 5%
3	C	248	 87% 10% .
3	Q	248	 85% 11% .
3	e	248	 83% 12% . .
3	s	248	 85% 10% . .
4	D	241	 86% 11% .
4	R	241	 86% 10% .
4	f	241	 88% 9% .
4	t	241	 90% 7% .
5	E	263	 82% 8% . 10%
5	S	263	 77% 13% . 10%
5	g	263	 80% 9% . 10%
5	u	263	 78% 13% 10%
6	F	255	 85% 11% .
6	T	255	 83% 12% . .
6	h	255	 87% 7% . .
6	v	255	 84% 11% .
7	G	246	 90% 9% .
7	U	246	 92% 7% .
7	i	246	 93% 6% .
7	w	246	 89% 10% .
8	H	234	 81% 13% 6%
8	V	234	 83% 10% . 6%


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	j	234	84% 10% 6%
8	x	234	83% 11% 6%
9	I	205	85% 13% .
9	W	205	92% 7%
9	k	205	90% 10%
9	y	205	86% 12% .
10	J	201	91% 6% ..
10	X	201	92% 6% .
10	l	201	94% . .
10	z	201	87% 10% ..
11	l	205	91% 7% .
11	K	205	91% 7% .
11	Y	205	92% 6% .
11	m	205	90% 8% .
12	2	213	90% 10%
12	L	213	86% 14%
12	Z	213	92% 8%
12	n	213	88% 12%
13	3	219	90% 7% ..
13	M	219	88% 11% .
13	a	219	89% 9% .
13	o	219	88% 10% ..
14	4	205	93% 5% .
14	N	205	92% 6% .
14	b	205	95% . .

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
14	p	205	 94% 5%

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 97956 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 type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	233	1817	1159	311	341	6	0	0	0
1	O	233	1817	1159	311	341	6	0	0	0
1	c	233	1817	1159	311	341	6	0	0	0
1	q	233	1817	1159	311	341	6	0	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	248	1950	1232	335	373	10	0	0	0
2	P	248	1950	1232	335	373	10	0	0	0
2	d	248	1950	1232	335	373	10	0	0	0
2	r	248	1950	1232	335	373	10	0	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	239	1881	1182	332	362	5	0	0	0
3	Q	239	1881	1182	332	362	5	0	0	0
3	e	239	1881	1182	332	362	5	0	0	0
3	s	239	1881	1182	332	362	5	0	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			
4	R	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			
4	f	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			
4	t	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			
5	S	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			
5	g	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			
5	u	238	Total	C	N	O	S	0	0	0
			1872	1171	336	354	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	T	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	h	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	v	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	0	0
			1895	1202	316	364	13			
7	U	244	Total	C	N	O	S	0	0	0
			1895	1202	316	364	13			
7	i	244	Total	C	N	O	S	0	0	0
			1895	1202	316	364	13			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	w	244	Total	C	N	O	S	0	0	0
			1895	1202	316	364	13			

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	V	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	j	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	x	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			
9	W	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			
9	k	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			
9	y	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	X	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	l	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	z	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	Y	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	m	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	1	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	n	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	2	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	a	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	o	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	3	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			
14	b	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			
14	p	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	4	202	1519	952	259	296	12	0	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	12	Total 12	O 12	0	0
15	B	11	Total 11	O 11	0	0
15	C	7	Total 7	O 7	0	0
15	D	5	Total 5	O 5	0	0
15	E	8	Total 8	O 8	0	0
15	F	11	Total 11	O 11	0	0
15	G	11	Total 11	O 11	0	0
15	H	17	Total 17	O 17	0	0
15	I	12	Total 12	O 12	0	0
15	J	13	Total 13	O 13	0	0
15	K	11	Total 11	O 11	0	0
15	L	18	Total 18	O 18	0	0
15	M	15	Total 15	O 15	0	0
15	N	13	Total 13	O 13	0	0
15	O	18	Total 18	O 18	0	0
15	P	24	Total 24	O 24	0	0
15	Q	12	Total 12	O 12	0	0
15	R	12	Total 12	O 12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	S	19	Total O 19 19	0	0
15	T	13	Total O 13 13	0	0
15	U	21	Total O 21 21	0	0
15	V	19	Total O 19 19	0	0
15	W	21	Total O 21 21	0	0
15	X	8	Total O 8 8	0	0
15	Y	8	Total O 8 8	0	0
15	Z	16	Total O 16 16	0	0
15	a	16	Total O 16 16	0	0
15	b	20	Total O 20 20	0	0
15	c	15	Total O 15 15	0	0
15	d	9	Total O 9 9	0	0
15	e	3	Total O 3 3	0	0
15	f	3	Total O 3 3	0	0
15	g	7	Total O 7 7	0	0
15	h	7	Total O 7 7	0	0
15	i	10	Total O 10 10	0	0
15	j	13	Total O 13 13	0	0
15	k	11	Total O 11 11	0	0
15	l	8	Total O 8 8	0	0
15	m	11	Total O 11 11	0	0

*Continued on next page...*

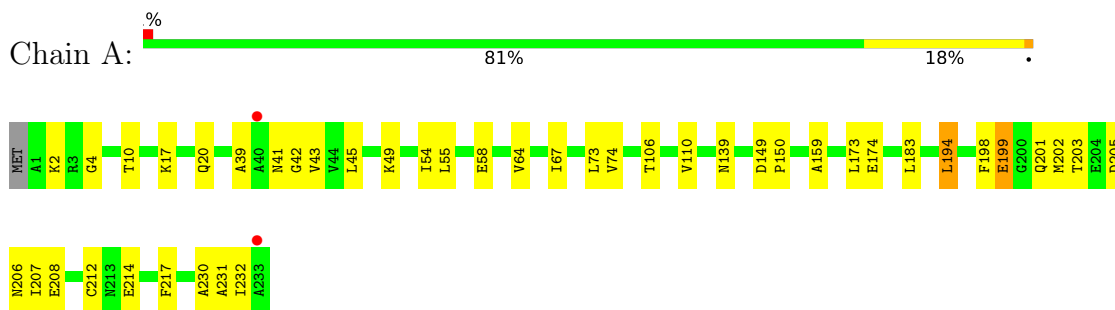
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	n	13	Total 13	O 13	0	0
15	o	11	Total 11	O 11	0	0
15	p	6	Total 6	O 6	0	0
15	q	3	Total 3	O 3	0	0
15	r	10	Total 10	O 10	0	0
15	s	7	Total 7	O 7	0	0
15	t	6	Total 6	O 6	0	0
15	u	7	Total 7	O 7	0	0
15	v	11	Total 11	O 11	0	0
15	w	10	Total 10	O 10	0	0
15	x	6	Total 6	O 6	0	0
15	y	10	Total 10	O 10	0	0
15	z	6	Total 6	O 6	0	0
15	1	12	Total 12	O 12	0	0
15	2	17	Total 17	O 17	0	0
15	3	10	Total 10	O 10	0	0
15	4	7	Total 7	O 7	0	0

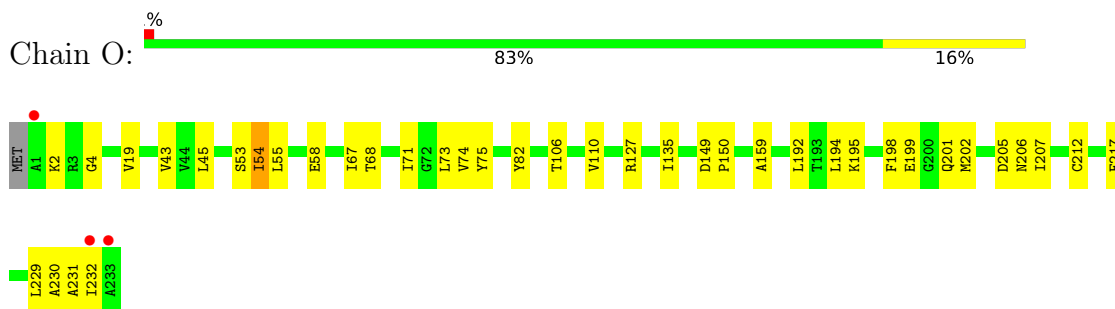
### 3 Residue-property plots [i](#)

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.

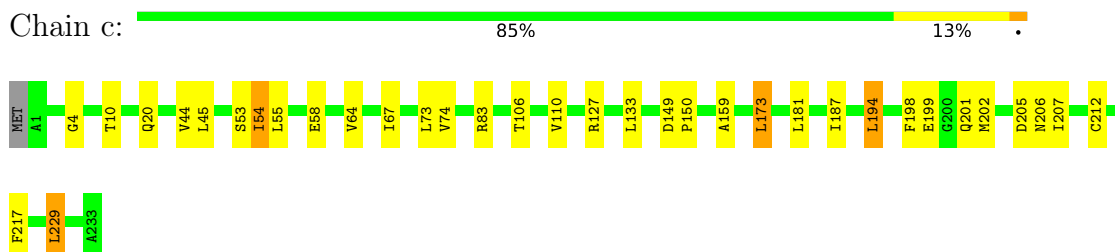
- Molecule 1: Proteasome subunit alpha type-2



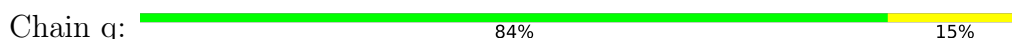
- Molecule 1: Proteasome subunit alpha type-2



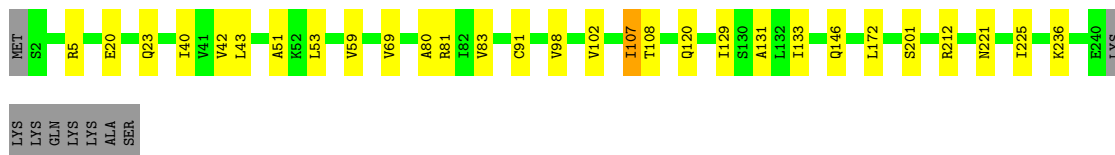
- Molecule 1: Proteasome subunit alpha type-2



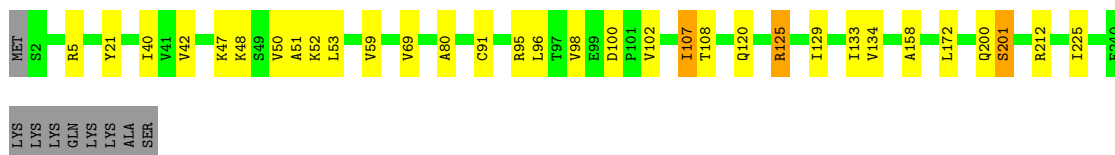
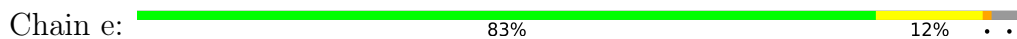
- Molecule 1: Proteasome subunit alpha type-2



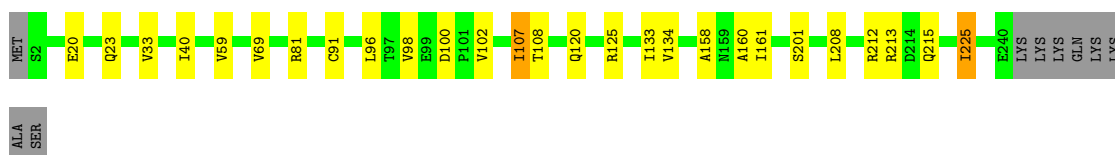
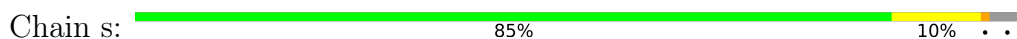




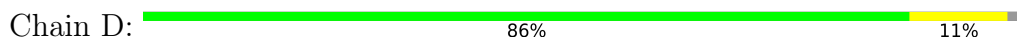
• Molecule 3: Proteasome subunit alpha type-7



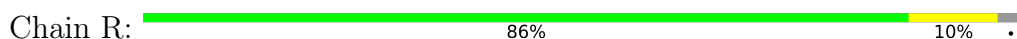
• Molecule 3: Proteasome subunit alpha type-7



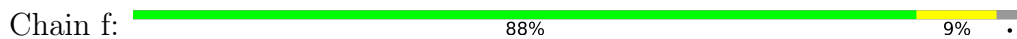
• Molecule 4: Proteasome subunit alpha type-5



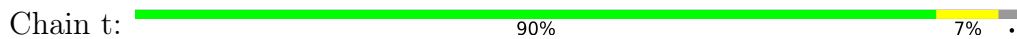
• Molecule 4: Proteasome subunit alpha type-5

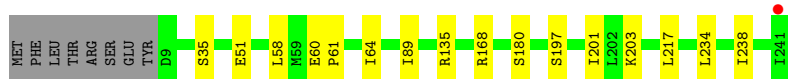


• Molecule 4: Proteasome subunit alpha type-5

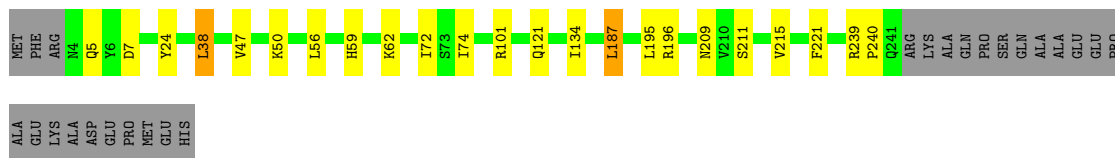
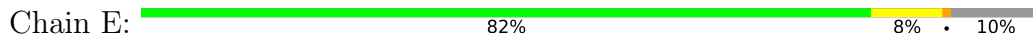


• Molecule 4: Proteasome subunit alpha type-5

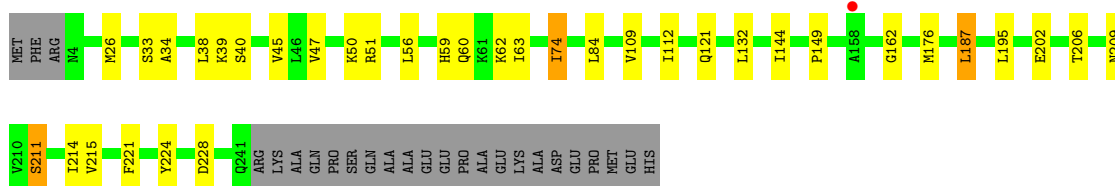




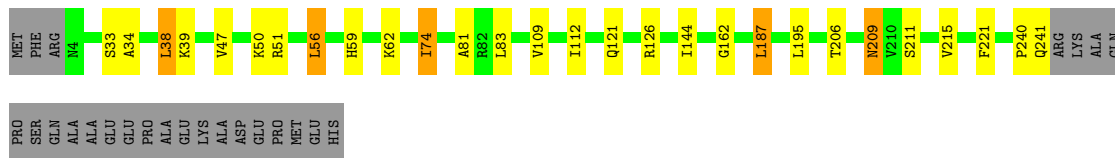
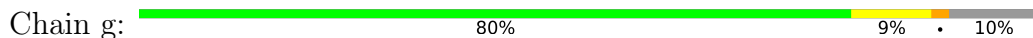
● Molecule 5: Proteasome subunit alpha type-1



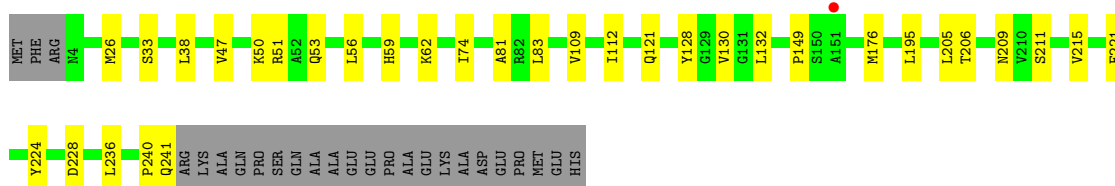
● Molecule 5: Proteasome subunit alpha type-1



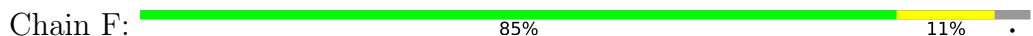
● Molecule 5: Proteasome subunit alpha type-1



● Molecule 5: Proteasome subunit alpha type-1

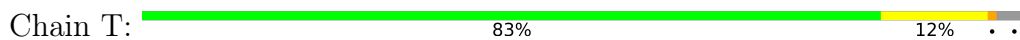


● Molecule 6: Proteasome subunit alpha type-3

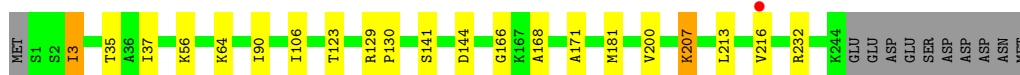
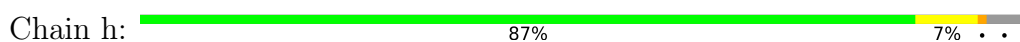


GLU  
SER  
ASP  
ASP  
ASP  
ASN  
MET

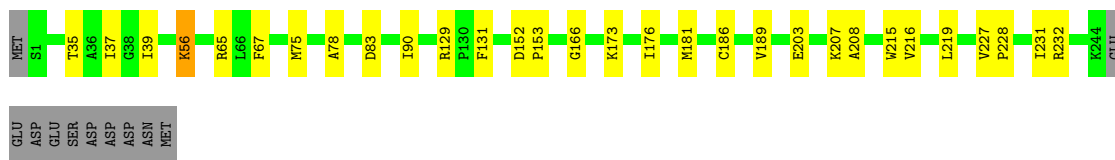
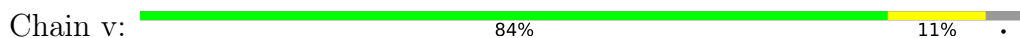
• Molecule 6: Proteasome subunit alpha type-3



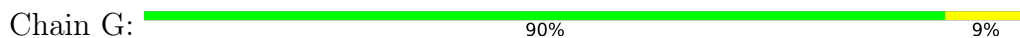
• Molecule 6: Proteasome subunit alpha type-3



• Molecule 6: Proteasome subunit alpha type-3



• Molecule 7: Proteasome subunit alpha type-6




• Molecule 7: Proteasome subunit alpha type-6



• Molecule 7: Proteasome subunit alpha type-6




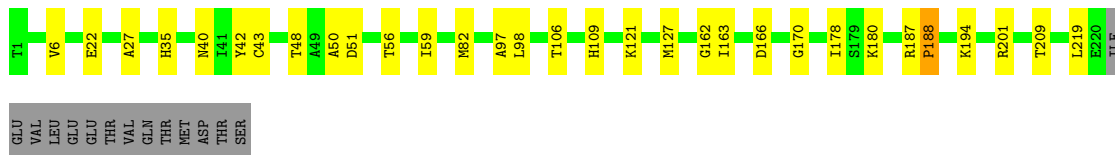
- Molecule 7: Proteasome subunit alpha type-6

Chain w:  89% 10%




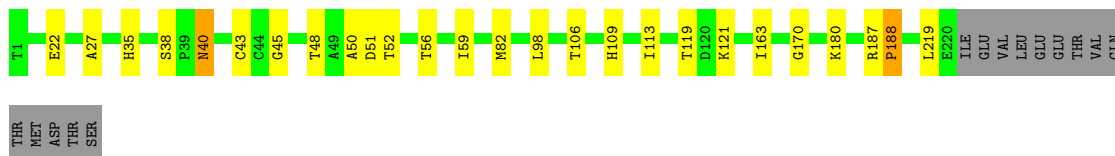
- Molecule 8: Proteasome subunit beta type-7

Chain H:  81% 13% 6%




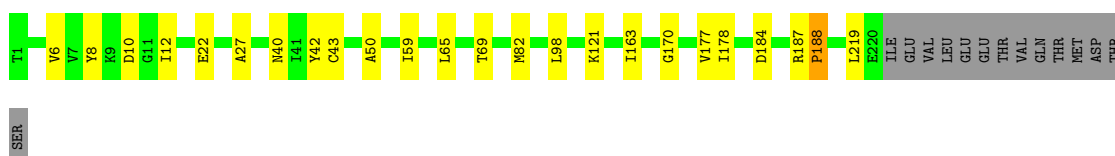
- Molecule 8: Proteasome subunit beta type-7

Chain V:  83% 10% 6%




- Molecule 8: Proteasome subunit beta type-7

Chain j:  84% 10% 6%




- Molecule 8: Proteasome subunit beta type-7

Chain x:  83% 11% 6%



- Molecule 9: Proteasome subunit beta type-3

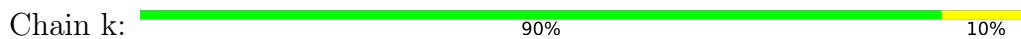
Chain I:  85% 13%



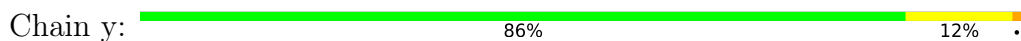
- Molecule 9: Proteasome subunit beta type-3



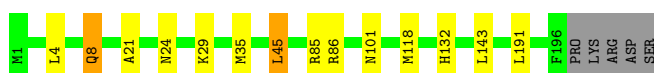
- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3



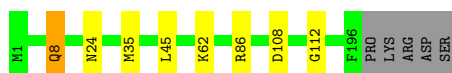
- Molecule 10: Proteasome subunit beta type-2



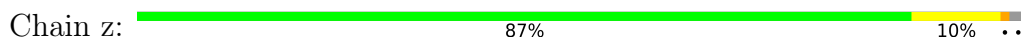
- Molecule 10: Proteasome subunit beta type-2

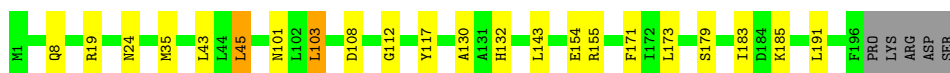


- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2





- Molecule 11: Proteasome subunit beta type-5



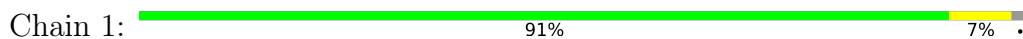
- Molecule 11: Proteasome subunit beta type-5



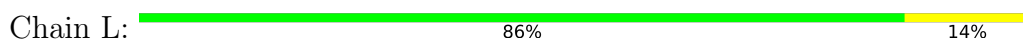
- Molecule 11: Proteasome subunit beta type-5



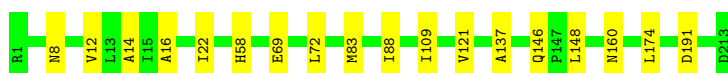
- Molecule 11: Proteasome subunit beta type-5



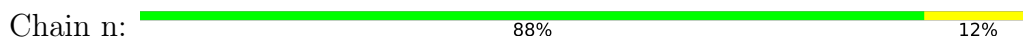
- Molecule 12: Proteasome subunit beta type-1



- Molecule 12: Proteasome subunit beta type-1

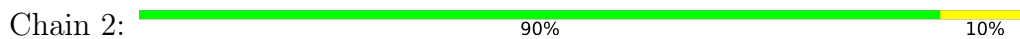


- Molecule 12: Proteasome subunit beta type-1

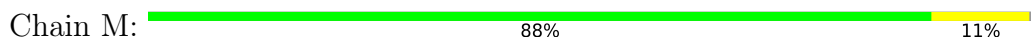




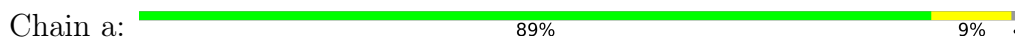
- Molecule 12: Proteasome subunit beta type-1



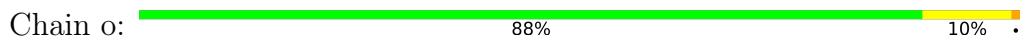
- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4



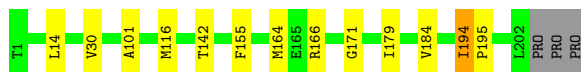
- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6





- Molecule 14: Proteasome subunit beta type-6

Chain p: 94% 5%



- Molecule 14: Proteasome subunit beta type-6

Chain 4: 93% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.97Å 201.30Å 226.01Å 90.00° 108.07° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-3.20) 97.3 (15.00-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.6.0119	Depositor
R, $R_{free}$	0.220 , 0.246 0.221 , 0.245	Depositor DCC
$R_{free}$ test set	11753 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.9	Xtrriage
Anisotropy	0.316	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 69.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	97956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.82% 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	0.52	0/1856	0.76	0/2512
1	O	0.52	0/1856	0.76	0/2512
1	c	0.52	0/1856	0.76	0/2512
1	q	0.52	0/1856	0.75	0/2512
2	B	0.49	0/1980	0.73	0/2667
2	P	0.49	0/1980	0.72	0/2667
2	d	0.49	0/1980	0.72	0/2667
2	r	0.49	0/1980	0.72	0/2667
3	C	0.46	0/1908	0.73	0/2576
3	Q	0.46	0/1908	0.75	0/2576
3	e	0.47	0/1908	0.74	0/2576
3	s	0.47	0/1908	0.73	0/2576
4	D	0.51	0/1805	0.73	0/2437
4	R	0.52	0/1805	0.74	0/2437
4	f	0.52	0/1805	0.73	0/2437
4	t	0.52	0/1805	0.72	0/2437
5	E	0.57	0/1907	0.74	0/2578
5	S	0.57	0/1907	0.74	0/2578
5	g	0.57	0/1907	0.71	0/2578
5	u	0.57	0/1907	0.74	0/2578
6	F	0.51	0/1938	0.71	0/2608
6	T	0.51	0/1938	0.72	0/2608
6	h	0.52	0/1938	0.71	0/2608
6	v	0.51	0/1938	0.72	0/2608
7	G	0.49	0/1929	0.73	0/2607
7	U	0.48	0/1929	0.73	0/2607
7	i	0.48	0/1929	0.73	0/2607
7	w	0.48	0/1929	0.74	0/2607
8	H	0.49	0/1683	0.72	0/2276
8	V	0.49	0/1683	0.74	0/2276
8	j	0.49	0/1683	0.73	0/2276
8	x	0.49	0/1683	0.72	0/2276
9	I	0.46	0/1621	0.73	0/2185
9	W	0.45	0/1621	0.73	0/2185

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	k	0.46	0/1621	0.72	0/2185
9	y	0.46	0/1621	0.71	0/2185
10	J	0.51	0/1602	0.69	0/2167
10	X	0.51	0/1602	0.69	0/2167
10	l	0.51	0/1602	0.70	0/2167
10	z	0.51	0/1602	0.70	0/2167
11	1	0.50	0/1588	0.68	0/2145
11	K	0.50	0/1588	0.69	0/2145
11	Y	0.50	0/1588	0.68	0/2145
11	m	0.50	0/1588	0.69	0/2145
12	2	0.48	0/1685	0.69	0/2271
12	L	0.48	0/1685	0.69	0/2271
12	Z	0.48	0/1685	0.70	0/2271
12	n	0.48	0/1685	0.69	0/2271
13	3	0.50	0/1718	0.69	0/2325
13	M	0.50	0/1718	0.71	0/2325
13	a	0.50	0/1718	0.70	0/2325
13	o	0.50	0/1718	0.70	0/2325
14	4	0.51	0/1546	0.73	1/2094 (0.0%)
14	N	0.51	0/1546	0.71	0/2094
14	b	0.51	0/1546	0.70	0/2094
14	p	0.52	0/1546	0.72	0/2094
All	All	0.50	0/99064	0.72	1/133792 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	190	LEU	N-CA-C	5.50	113.29	108.78

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	A	1817	0	1812	21	0
1	O	1817	0	1812	18	0
1	c	1817	0	1812	18	0
1	q	1817	0	1812	15	0
2	B	1950	0	1970	7	0
2	P	1950	0	1970	5	0
2	d	1950	0	1970	11	0
2	r	1950	0	1970	4	0
3	C	1881	0	1901	10	0
3	Q	1881	0	1901	12	0
3	e	1881	0	1901	14	0
3	s	1881	0	1901	14	0
4	D	1778	0	1764	12	0
4	R	1778	0	1764	14	0
4	f	1778	0	1764	12	0
4	t	1778	0	1764	8	0
5	E	1872	0	1856	11	0
5	S	1872	0	1856	18	0
5	g	1872	0	1856	15	0
5	u	1872	0	1856	16	0
6	F	1903	0	1894	11	0
6	T	1903	0	1894	14	0
6	h	1903	0	1894	8	0
6	v	1903	0	1894	15	0
7	G	1895	0	1899	12	0
7	U	1895	0	1899	9	0
7	i	1895	0	1899	7	0
7	w	1895	0	1899	13	0
8	H	1656	0	1685	17	0
8	V	1656	0	1685	13	0
8	j	1656	0	1685	12	0
8	x	1656	0	1685	12	0
9	I	1592	0	1612	15	0
9	W	1592	0	1612	6	0
9	k	1592	0	1612	10	0
9	y	1592	0	1612	12	0
10	J	1570	0	1573	7	0
10	X	1570	0	1573	5	0
10	l	1570	0	1573	5	0
10	z	1570	0	1573	8	0
11	l	1557	0	1526	5	0
11	K	1557	0	1526	6	0
11	Y	1557	0	1526	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	m	1557	0	1526	7	0
12	2	1654	0	1652	9	0
12	L	1654	0	1652	11	0
12	Z	1654	0	1652	8	0
12	n	1654	0	1652	12	0
13	3	1685	0	1664	11	0
13	M	1685	0	1664	11	0
13	a	1685	0	1664	12	0
13	o	1685	0	1664	11	0
14	4	1519	0	1488	8	0
14	N	1519	0	1488	8	0
14	b	1519	0	1488	6	0
14	p	1519	0	1488	5	0
15	1	12	0	0	0	0
15	2	17	0	0	0	0
15	3	10	0	0	0	0
15	4	7	0	0	0	0
15	A	12	0	0	0	0
15	B	11	0	0	0	0
15	C	7	0	0	0	0
15	D	5	0	0	0	0
15	E	8	0	0	0	0
15	F	11	0	0	0	0
15	G	11	0	0	0	0
15	H	17	0	0	0	0
15	I	12	0	0	0	0
15	J	13	0	0	0	0
15	K	11	0	0	0	0
15	L	18	0	0	0	0
15	M	15	0	0	0	0
15	N	13	0	0	0	0
15	O	18	0	0	0	0
15	P	24	0	0	0	0
15	Q	12	0	0	0	0
15	R	12	0	0	0	0
15	S	19	0	0	0	0
15	T	13	0	0	0	0
15	U	21	0	0	0	0
15	V	19	0	0	0	0
15	W	21	0	0	0	0
15	X	8	0	0	0	0
15	Y	8	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Z	16	0	0	0	0
15	a	16	0	0	0	0
15	b	20	0	0	0	0
15	c	15	0	0	0	0
15	d	9	0	0	0	0
15	e	3	0	0	0	0
15	f	3	0	0	0	0
15	g	7	0	0	0	0
15	h	7	0	0	0	0
15	i	10	0	0	0	0
15	j	13	0	0	0	0
15	k	11	0	0	0	0
15	l	8	0	0	0	0
15	m	11	0	0	0	0
15	n	13	0	0	0	0
15	o	11	0	0	0	0
15	p	6	0	0	0	0
15	q	3	0	0	0	0
15	r	10	0	0	0	0
15	s	7	0	0	0	0
15	t	6	0	0	0	0
15	u	7	0	0	0	0
15	v	11	0	0	0	0
15	w	10	0	0	0	0
15	x	6	0	0	0	0
15	y	10	0	0	0	0
15	z	6	0	0	0	0
All	All	97956	0	97184	525	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 3.

The worst 5 of 525 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:4:GLY:HA2	7:w:130:GLU:HG2	1.63	0.81
8:x:187:ARG:HB3	8:x:188:PRO:HD3	1.64	0.80
1:A:4:GLY:HA2	7:G:130:GLU:HG2	1.64	0.78
8:j:187:ARG:HB3	8:j:188:PRO:HD3	1.65	0.77
8:H:187:ARG:HB3	8:H:188:PRO:HD3	1.67	0.77

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	231/234 (99%)	213 (92%)	14 (6%)	4 (2%)	7	35
1	O	231/234 (99%)	217 (94%)	11 (5%)	3 (1%)	9	40
1	c	231/234 (99%)	213 (92%)	14 (6%)	4 (2%)	7	35
1	q	231/234 (99%)	213 (92%)	12 (5%)	6 (3%)	4	26
2	B	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	30	62
2	P	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	30	62
2	d	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	30	62
2	r	246/261 (94%)	239 (97%)	6 (2%)	1 (0%)	30	62
3	C	237/248 (96%)	226 (95%)	10 (4%)	1 (0%)	30	62
3	Q	237/248 (96%)	229 (97%)	7 (3%)	1 (0%)	30	62
3	e	237/248 (96%)	227 (96%)	8 (3%)	2 (1%)	16	50
3	s	237/248 (96%)	230 (97%)	6 (2%)	1 (0%)	30	62
4	D	231/241 (96%)	219 (95%)	12 (5%)	0	100	100
4	R	231/241 (96%)	219 (95%)	12 (5%)	0	100	100
4	f	231/241 (96%)	218 (94%)	13 (6%)	0	100	100
4	t	231/241 (96%)	217 (94%)	14 (6%)	0	100	100
5	E	236/263 (90%)	228 (97%)	7 (3%)	1 (0%)	30	62
5	S	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
5	g	236/263 (90%)	227 (96%)	8 (3%)	1 (0%)	30	62
5	u	236/263 (90%)	224 (95%)	11 (5%)	1 (0%)	30	62
6	F	242/255 (95%)	229 (95%)	11 (4%)	2 (1%)	16	50
6	T	242/255 (95%)	228 (94%)	12 (5%)	2 (1%)	16	50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	h	242/255 (95%)	230 (95%)	10 (4%)	2 (1%)	16	50
6	v	242/255 (95%)	229 (95%)	12 (5%)	1 (0%)	30	62
7	G	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
7	U	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
7	i	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	62
7	w	242/246 (98%)	232 (96%)	9 (4%)	1 (0%)	30	62
8	H	218/234 (93%)	204 (94%)	13 (6%)	1 (0%)	24	59
8	V	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	24	59
8	j	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	24	59
8	x	218/234 (93%)	204 (94%)	13 (6%)	1 (0%)	24	59
9	I	202/205 (98%)	187 (93%)	8 (4%)	7 (4%)	3	20
9	W	202/205 (98%)	189 (94%)	9 (4%)	4 (2%)	6	31
9	k	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	8	37
9	y	202/205 (98%)	186 (92%)	13 (6%)	3 (2%)	8	37
10	J	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	24	59
10	X	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	24	59
10	l	194/201 (96%)	182 (94%)	11 (6%)	1 (0%)	24	59
10	z	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	24	59
11	1	199/205 (97%)	188 (94%)	11 (6%)	0	100	100
11	K	199/205 (97%)	188 (94%)	11 (6%)	0	100	100
11	Y	199/205 (97%)	190 (96%)	9 (4%)	0	100	100
11	m	199/205 (97%)	190 (96%)	9 (4%)	0	100	100
12	2	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	24	59
12	L	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	24	59
12	Z	211/213 (99%)	203 (96%)	7 (3%)	1 (0%)	24	59
12	n	211/213 (99%)	201 (95%)	9 (4%)	1 (0%)	24	59
13	3	214/219 (98%)	203 (95%)	11 (5%)	0	100	100
13	M	214/219 (98%)	204 (95%)	10 (5%)	0	100	100
13	a	214/219 (98%)	204 (95%)	10 (5%)	0	100	100
13	o	214/219 (98%)	202 (94%)	12 (6%)	0	100	100
14	4	200/205 (98%)	187 (94%)	13 (6%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	200/205 (98%)	192 (96%)	8 (4%)	0	100	100
14	b	200/205 (98%)	191 (96%)	9 (4%)	0	100	100
14	p	200/205 (98%)	188 (94%)	11 (6%)	1 (0%)	24	59
All	All	12412/12920 (96%)	11795 (95%)	549 (4%)	68 (0%)	24	59

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
9	I	116	PHE
10	J	24	ASN
1	O	201	GLN
10	X	24	ASN

### 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	189/191 (99%)	183 (97%)	6 (3%)	34	65
1	O	189/191 (99%)	181 (96%)	8 (4%)	26	60
1	c	189/191 (99%)	182 (96%)	7 (4%)	30	63
1	q	189/191 (99%)	184 (97%)	5 (3%)	40	69
2	B	208/221 (94%)	202 (97%)	6 (3%)	37	67
2	P	208/221 (94%)	200 (96%)	8 (4%)	29	62
2	d	208/221 (94%)	201 (97%)	7 (3%)	32	64
2	r	208/221 (94%)	198 (95%)	10 (5%)	23	56
3	C	202/211 (96%)	193 (96%)	9 (4%)	24	58
3	Q	202/211 (96%)	193 (96%)	9 (4%)	24	58
3	e	202/211 (96%)	192 (95%)	10 (5%)	22	55
3	s	202/211 (96%)	195 (96%)	7 (4%)	32	64
4	D	195/203 (96%)	188 (96%)	7 (4%)	31	63

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	195/203 (96%)	190 (97%)	5 (3%)	40	69
4	f	195/203 (96%)	190 (97%)	5 (3%)	40	69
4	t	195/203 (96%)	191 (98%)	4 (2%)	47	71
5	E	204/224 (91%)	197 (97%)	7 (3%)	32	64
5	S	204/224 (91%)	195 (96%)	9 (4%)	25	59
5	g	204/224 (91%)	196 (96%)	8 (4%)	28	62
5	u	204/224 (91%)	198 (97%)	6 (3%)	37	67
6	F	200/211 (95%)	193 (96%)	7 (4%)	32	64
6	T	200/211 (95%)	192 (96%)	8 (4%)	28	61
6	h	200/211 (95%)	192 (96%)	8 (4%)	28	61
6	v	200/211 (95%)	194 (97%)	6 (3%)	36	66
7	G	207/210 (99%)	203 (98%)	4 (2%)	50	73
7	U	207/210 (99%)	201 (97%)	6 (3%)	37	67
7	i	207/210 (99%)	202 (98%)	5 (2%)	43	70
7	w	207/210 (99%)	200 (97%)	7 (3%)	32	64
8	H	181/195 (93%)	175 (97%)	6 (3%)	33	65
8	V	181/195 (93%)	178 (98%)	3 (2%)	53	75
8	j	181/195 (93%)	176 (97%)	5 (3%)	38	68
8	x	181/195 (93%)	175 (97%)	6 (3%)	33	65
9	I	174/175 (99%)	171 (98%)	3 (2%)	53	75
9	W	174/175 (99%)	170 (98%)	4 (2%)	44	70
9	k	174/175 (99%)	171 (98%)	3 (2%)	53	75
9	y	174/175 (99%)	168 (97%)	6 (3%)	32	64
10	J	166/171 (97%)	162 (98%)	4 (2%)	43	70
10	X	166/171 (97%)	162 (98%)	4 (2%)	43	70
10	l	166/171 (97%)	165 (99%)	1 (1%)	78	84
10	z	166/171 (97%)	158 (95%)	8 (5%)	23	56
11	l	157/161 (98%)	152 (97%)	5 (3%)	34	65
11	K	157/161 (98%)	153 (98%)	4 (2%)	42	69
11	Y	157/161 (98%)	152 (97%)	5 (3%)	34	65
11	m	157/161 (98%)	152 (97%)	5 (3%)	34	65

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	2	178/178 (100%)	171 (96%)	7 (4%)	28	62
12	L	178/178 (100%)	170 (96%)	8 (4%)	24	58
12	Z	178/178 (100%)	175 (98%)	3 (2%)	53	75
12	n	178/178 (100%)	172 (97%)	6 (3%)	32	64
13	3	178/180 (99%)	174 (98%)	4 (2%)	45	71
13	M	178/180 (99%)	175 (98%)	3 (2%)	53	75
13	a	178/180 (99%)	175 (98%)	3 (2%)	53	75
13	o	178/180 (99%)	172 (97%)	6 (3%)	32	64
14	4	159/162 (98%)	159 (100%)	0	100	100
14	N	159/162 (98%)	157 (99%)	2 (1%)	61	78
14	b	159/162 (98%)	158 (99%)	1 (1%)	78	84
14	p	159/162 (98%)	157 (99%)	2 (1%)	61	78
All	All	10392/10772 (96%)	10081 (97%)	311 (3%)	36	66

5 of 311 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	q	43	VAL
9	y	171	LEU
2	r	164	ILE
5	u	205	LEU
12	2	62	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 218 such sidechains are listed below:

Mol	Chain	Res	Type
2	d	100	GLN
10	l	61	GLN
11	1	38	ASN
3	e	205	ASN
7	i	127	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	233/234 (99%)	-0.10	2 (0%) 81 64	68, 101, 151, 178	0
1	O	233/234 (99%)	-0.27	3 (1%) 75 55	56, 79, 133, 166	0
1	c	233/234 (99%)	-0.26	0 100 100	75, 107, 157, 181	0
1	q	233/234 (99%)	-0.22	1 (0%) 88 79	80, 107, 155, 173	0
2	B	248/261 (95%)	-0.33	0 100 100	65, 95, 143, 169	0
2	P	248/261 (95%)	-0.38	0 100 100	51, 78, 117, 157	0
2	d	248/261 (95%)	-0.31	1 (0%) 88 79	65, 110, 164, 202	0
2	r	248/261 (95%)	-0.31	0 100 100	78, 110, 148, 167	0
3	C	239/248 (96%)	-0.23	2 (0%) 82 67	73, 109, 169, 202	0
3	Q	239/248 (96%)	-0.28	0 100 100	61, 98, 156, 197	0
3	e	239/248 (96%)	-0.22	0 100 100	80, 125, 178, 204	0
3	s	239/248 (96%)	-0.20	0 100 100	91, 125, 174, 196	0
4	D	233/241 (96%)	-0.29	0 100 100	59, 96, 130, 154	0
4	R	233/241 (96%)	-0.35	0 100 100	67, 101, 139, 176	0
4	f	233/241 (96%)	-0.27	0 100 100	77, 124, 155, 185	0
4	t	233/241 (96%)	-0.28	1 (0%) 88 79	71, 120, 157, 190	0
5	E	238/263 (90%)	-0.34	0 100 100	57, 93, 148, 178	0
5	S	238/263 (90%)	-0.25	1 (0%) 88 79	66, 98, 154, 184	0
5	g	238/263 (90%)	-0.14	0 100 100	81, 117, 163, 192	0
5	u	238/263 (90%)	-0.26	1 (0%) 88 79	66, 108, 162, 182	0
6	F	244/255 (95%)	-0.28	0 100 100	63, 97, 146, 162	0
6	T	244/255 (95%)	-0.29	0 100 100	58, 89, 143, 168	0
6	h	244/255 (95%)	-0.19	1 (0%) 88 79	87, 121, 165, 179	0
6	v	244/255 (95%)	-0.27	0 100 100	81, 109, 149, 169	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	G	244/246 (99%)	-0.28	0 100 100	66, 101, 149, 170	0
7	U	244/246 (99%)	-0.35	0 100 100	57, 81, 114, 144	0
7	i	244/246 (99%)	-0.24	0 100 100	81, 121, 159, 180	0
7	w	244/246 (99%)	-0.22	0 100 100	78, 107, 150, 169	0
8	H	220/234 (94%)	-0.24	0 100 100	62, 81, 130, 169	0
8	V	220/234 (94%)	-0.38	0 100 100	49, 65, 103, 153	0
8	j	220/234 (94%)	-0.32	0 100 100	71, 87, 125, 151	0
8	x	220/234 (94%)	-0.23	0 100 100	69, 93, 142, 175	0
9	I	204/205 (99%)	-0.29	0 100 100	64, 79, 118, 146	0
9	W	204/205 (99%)	-0.44	1 (0%) 87 76	52, 66, 96, 129	0
9	k	204/205 (99%)	-0.35	0 100 100	69, 84, 120, 141	0
9	y	204/205 (99%)	-0.19	0 100 100	75, 100, 146, 156	0
10	J	196/201 (97%)	-0.41	0 100 100	58, 75, 104, 124	0
10	X	196/201 (97%)	-0.42	0 100 100	53, 70, 99, 132	0
10	l	196/201 (97%)	-0.35	0 100 100	66, 92, 122, 146	0
10	z	196/201 (97%)	-0.35	0 100 100	70, 95, 130, 158	0
11	1	201/205 (98%)	-0.38	0 100 100	60, 86, 119, 147	0
11	K	201/205 (98%)	-0.39	0 100 100	53, 70, 102, 123	0
11	Y	201/205 (98%)	-0.37	1 (0%) 87 76	59, 77, 106, 137	0
11	m	201/205 (98%)	-0.27	0 100 100	69, 95, 130, 159	0
12	2	213/213 (100%)	-0.36	0 100 100	66, 84, 110, 157	0
12	L	213/213 (100%)	-0.41	0 100 100	53, 68, 98, 146	0
12	Z	213/213 (100%)	-0.28	0 100 100	56, 84, 125, 172	0
12	n	213/213 (100%)	-0.26	0 100 100	75, 102, 138, 166	0
13	3	216/219 (98%)	-0.40	0 100 100	65, 82, 112, 153	0
13	M	216/219 (98%)	-0.39	0 100 100	54, 70, 99, 119	0
13	a	216/219 (98%)	-0.33	0 100 100	53, 75, 106, 129	0
13	o	216/219 (98%)	-0.34	0 100 100	64, 91, 122, 132	0
14	4	202/205 (98%)	-0.38	0 100 100	61, 86, 125, 159	0
14	N	202/205 (98%)	-0.39	0 100 100	47, 74, 112, 157	0
14	b	202/205 (98%)	-0.40	0 100 100	55, 69, 113, 160	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	p	202/205 (98%)	-0.30	0 100 100	68, 89, 139, 164	0
All	All	12524/12920 (96%)	-0.30	15 (0%) 92 89	47, 93, 150, 204	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	ALA	2.9
5	u	151	ALA	2.8
1	O	233	ALA	2.7
5	S	158	ALA	2.6
3	C	46	GLU	2.5

## 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.