



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:40 PM BST

PDB ID : 3UNE  
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 Full wwPDB X-ray Structure Validation 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13



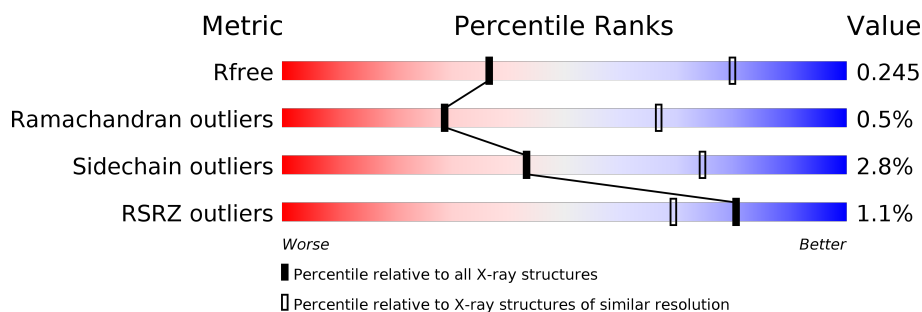
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	1133 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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	<div> <div>%</div> <div>96%</div> <div>.</div> </div>
1	O	234	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
1	c	234	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	q	234	<div> <div>%</div> <div>94%</div> <div>6%</div> </div>
2	B	261	<div> <div>%</div> <div>92%</div> <div>5%</div> </div>
2	P	261	<div> <div>%</div> <div>92%</div> <div>5%</div> </div>
2	d	261	<div> <div>5%</div> <div>92%</div> <div>5%</div> </div>

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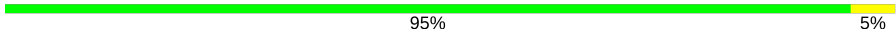
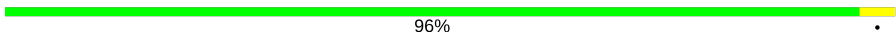
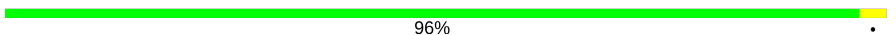
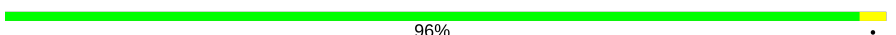

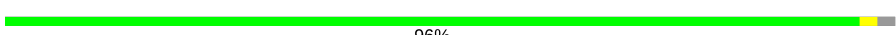









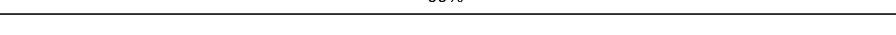
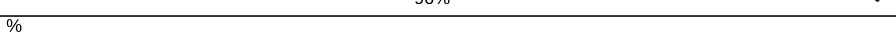
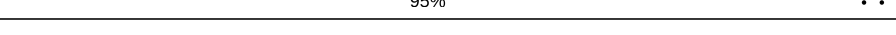
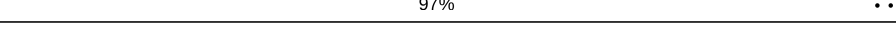
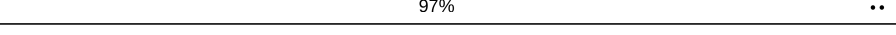
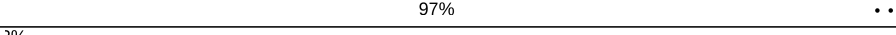
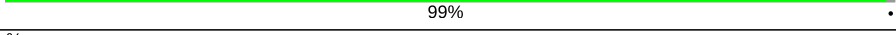
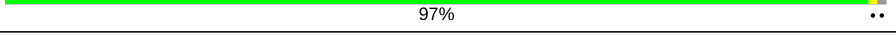
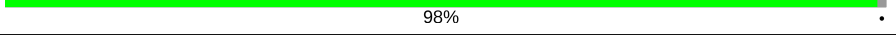
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Mol	Chain	Length	Quality of chain
2	r	261	
3	C	248	
3	Q	248	
3	e	248	
3	s	248	
4	D	241	
4	R	241	
4	f	241	
4	t	241	
5	E	263	
5	S	263	
5	g	263	
5	u	263	
6	F	255	
6	T	255	
6	h	255	
6	v	255	
7	G	246	
7	U	246	
7	i	246	
7	w	246	
8	H	234	
8	V	234	
8	j	234	
8	x	234	

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Mol	Chain	Length	Quality of chain
9	I	205	 95%5%
9	W	205	 96%.
9	k	205	 96%.
9	y	205	 96%.
10	J	201	 95%..
10	X	201	 96%..
10	l	201	 97%..
10	z	201	 94%..
11	1	205	 97%..
11	K	205	 97%..
11	Y	205	 97%..
11	m	205	 96%..
12	2	213	 96%.
12	L	213	 96%.
12	Z	213	 99%.
12	n	213	 96%.
13	3	219	 95%..
13	M	219	 97%..
13	a	219	 97%..
13	o	219	 97%..
14	4	205	 99%.
14	N	205	 97%..
14	b	205	 98%.
14	p	205	 97%..



## 2 Entry composition

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
1	A	233	Total	C	N	O	S	0	0	0
			1817	1159	311	341	6			
1	O	233	Total	C	N	O	S	0	0	0
			1817	1159	311	341	6			
1	c	233	Total	C	N	O	S	0	0	0
			1817	1159	311	341	6			
1	q	233	Total	C	N	O	S	0	0	0
			1817	1159	311	341	6			

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

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

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

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



- 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			

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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			

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

- Molecule 15 is water.

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

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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

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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.

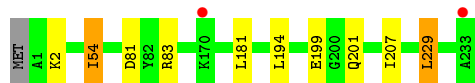
- Molecule 1: Proteasome subunit alpha type-2



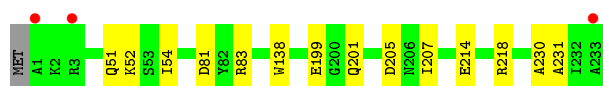
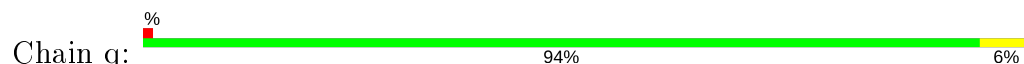
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2

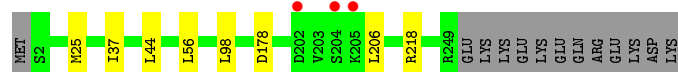


- Molecule 2: Proteasome subunit alpha type-4



- Molecule 2: Proteasome subunit alpha type-4

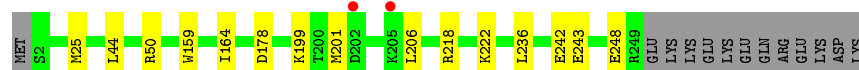
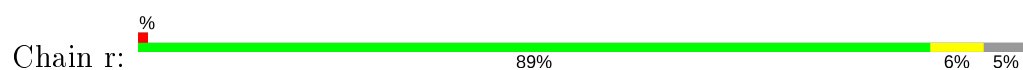




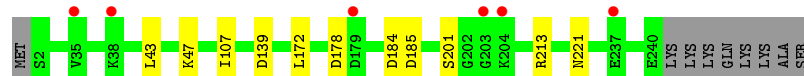
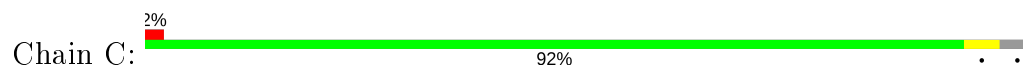
- Molecule 2: Proteasome subunit alpha type-4



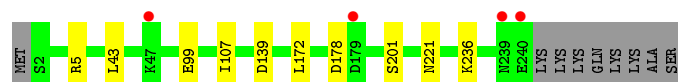
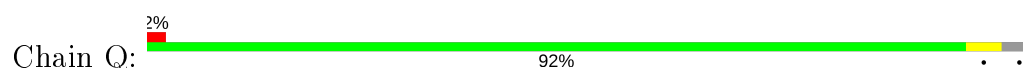
- Molecule 2: Proteasome subunit alpha type-4



- Molecule 3: Proteasome subunit alpha type-7



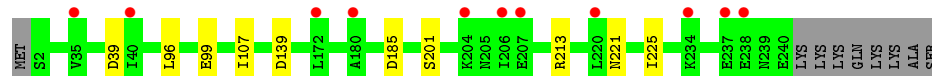
- Molecule 3: Proteasome subunit alpha type-7



- Molecule 3: Proteasome subunit alpha type-7



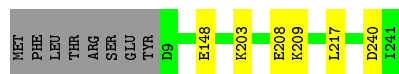
- Molecule 3: Proteasome subunit alpha type-7





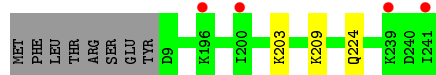
- Molecule 4: Proteasome subunit alpha type-5

Chain D:  94% ..



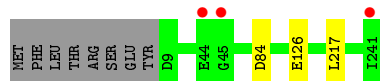
- Molecule 4: Proteasome subunit alpha type-5

Chain R:  95% ..



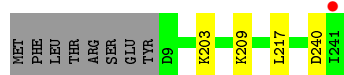
- Molecule 4: Proteasome subunit alpha type-5

Chain f:  95% ..




- Molecule 4: Proteasome subunit alpha type-5

Chain t:  95% ..




- Molecule 5: Proteasome subunit alpha type-1

Chain E:  87% 10%



- Molecule 5: Proteasome subunit alpha type-1

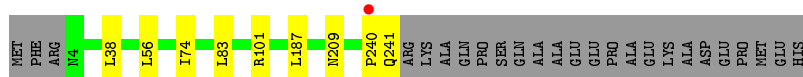
Chain S:  87% 10%



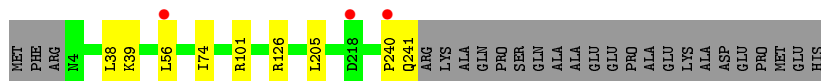
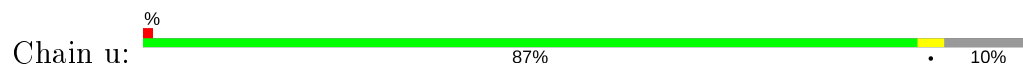
- Molecule 5: Proteasome subunit alpha type-1

Chain g:  87% 10%

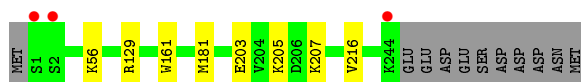




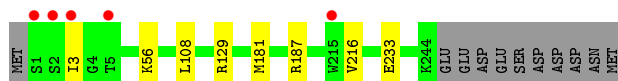
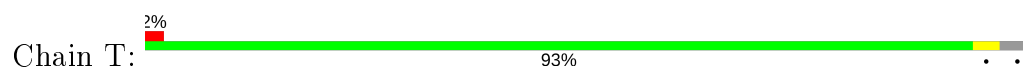
- Molecule 5: Proteasome subunit alpha type-1



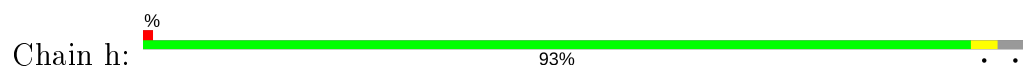
- Molecule 6: Proteasome subunit alpha type-3



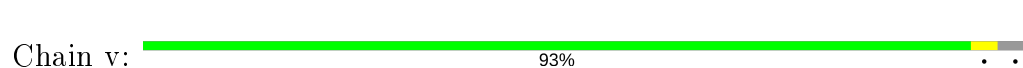
- Molecule 6: Proteasome subunit alpha type-3



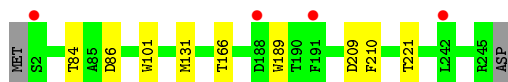
- Molecule 6: Proteasome subunit alpha type-3



- Molecule 6: Proteasome subunit alpha type-3



- Molecule 7: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-6

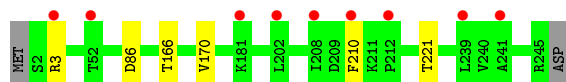


Chain U:  96%




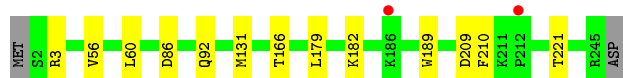
- Molecule 7: Proteasome subunit alpha type-6

Chain i:  97%



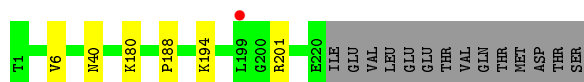
- Molecule 7: Proteasome subunit alpha type-6

Chain w:  94%



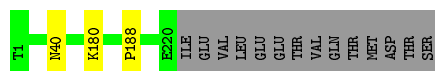
- Molecule 8: Proteasome subunit beta type-7

Chain H:  91%



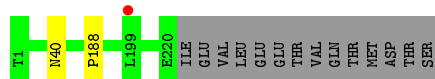
- Molecule 8: Proteasome subunit beta type-7

Chain V:  93%



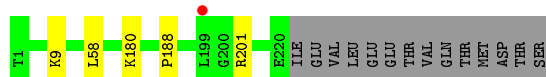
- Molecule 8: Proteasome subunit beta type-7

Chain j:  93%



- Molecule 8: Proteasome subunit beta type-7

Chain x:  92%





- Molecule 9: Proteasome subunit beta type-3

Chain I:  95% 5%



- Molecule 9: Proteasome subunit beta type-3

Chain W:  96% .



- Molecule 9: Proteasome subunit beta type-3

Chain k:  96% .



- Molecule 9: Proteasome subunit beta type-3

Chain y:  96% .



- Molecule 10: Proteasome subunit beta type-2

Chain J:  95% ..



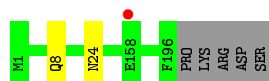
- Molecule 10: Proteasome subunit beta type-2

Chain X:  96% ..



- Molecule 10: Proteasome subunit beta type-2

Chain l:  97% ..





- Molecule 10: Proteasome subunit beta type-2

Chain z:  94% ..



- Molecule 11: Proteasome subunit beta type-5

Chain K:  97% ..



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  97% ..



- Molecule 11: Proteasome subunit beta type-5

Chain m:  96% ..



- Molecule 11: Proteasome subunit beta type-5

Chain 1:  97% ..



- Molecule 12: Proteasome subunit beta type-1

Chain L:  96% .



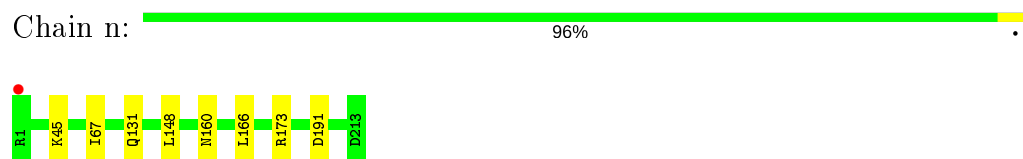
- Molecule 12: Proteasome subunit beta type-1

Chain Z:  99% .

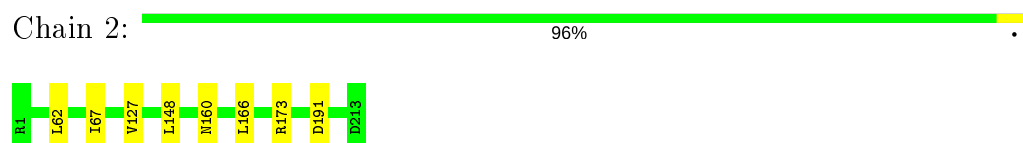




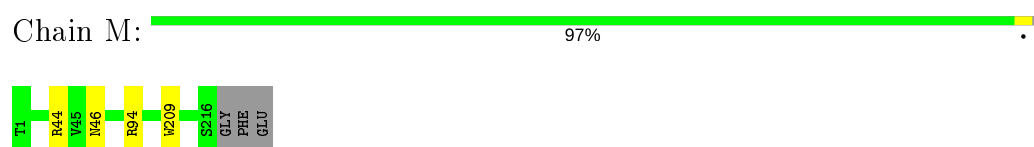
- Molecule 12: Proteasome subunit beta type-1



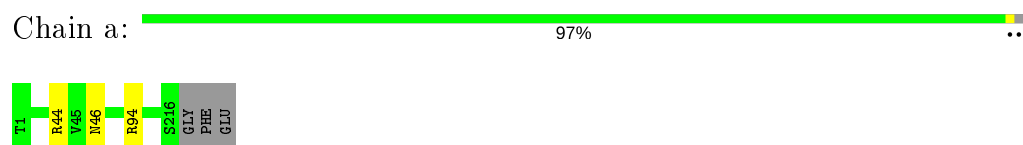
- Molecule 12: Proteasome subunit beta type-1



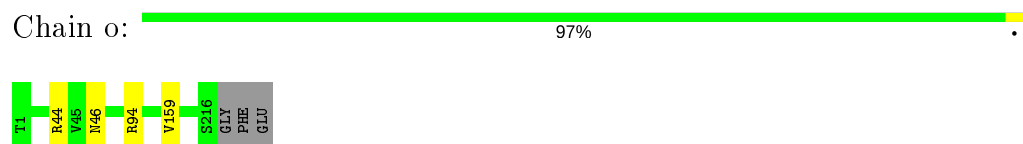
- Molecule 13: Proteasome subunit beta type-4



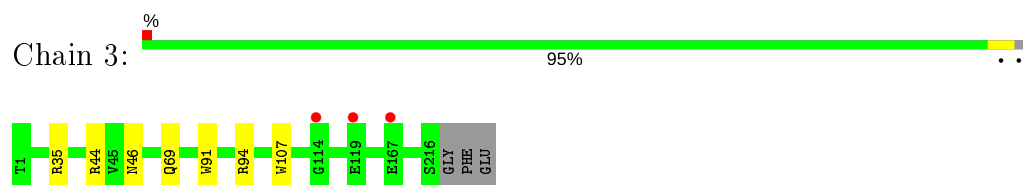
- Molecule 13: Proteasome subunit beta type-4



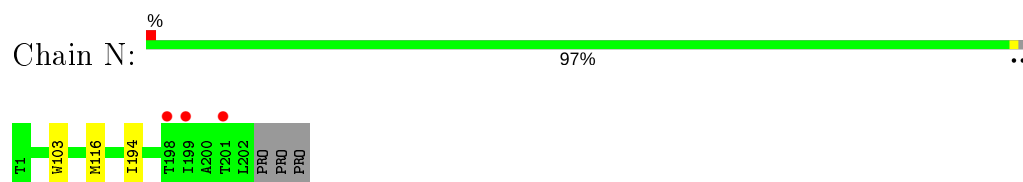
- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4

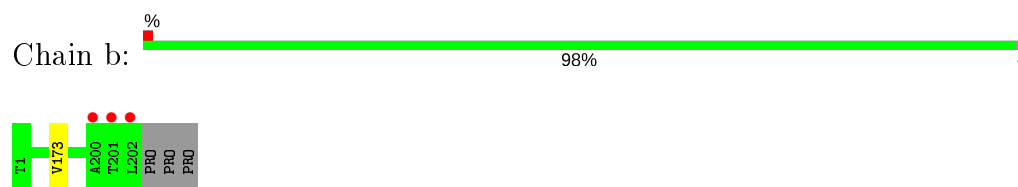


- Molecule 14: Proteasome subunit beta type-6

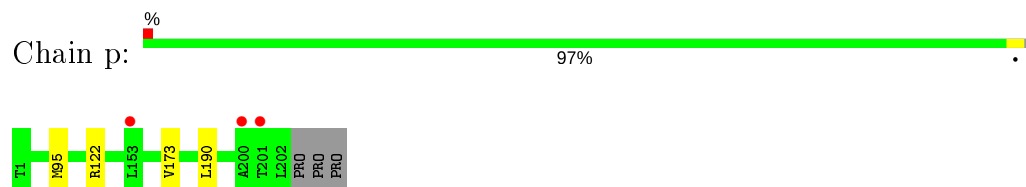




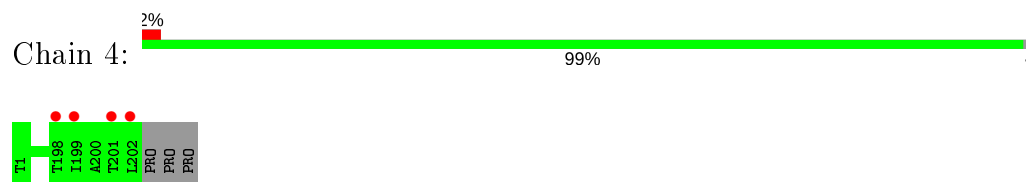
- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6





## 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 49.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-3.20) 98.0 (49.90-3.20)	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)	Xtriage
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	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	97956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage'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

### 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	0.38	1/1856 (0.1%)	0.45	0/2512
1	O	0.38	1/1856 (0.1%)	0.46	0/2512
1	c	0.38	0/1856	0.46	0/2512
1	q	0.39	1/1856 (0.1%)	0.45	0/2512
2	B	0.37	0/1980	0.45	0/2667
2	P	0.36	0/1980	0.45	0/2667
2	d	0.37	1/1980 (0.1%)	0.45	0/2667
2	r	0.37	1/1980 (0.1%)	0.45	0/2667
3	C	0.33	0/1908	0.45	0/2576
3	Q	0.33	0/1908	0.45	0/2576
3	e	0.33	1/1908 (0.1%)	0.46	0/2576
3	s	0.33	0/1908	0.44	0/2576
4	D	0.35	0/1805	0.44	0/2437
4	R	0.36	0/1805	0.44	0/2437
4	f	0.35	0/1805	0.44	0/2437
4	t	0.35	0/1805	0.44	0/2437
5	E	0.37	1/1907 (0.1%)	0.45	0/2578
5	S	0.37	0/1907	0.46	0/2578
5	g	0.37	0/1907	0.46	0/2578
5	u	0.37	0/1907	0.46	0/2578
6	F	0.38	1/1938 (0.1%)	0.43	0/2608
6	T	0.38	0/1938	0.44	0/2608
6	h	0.38	0/1938	0.44	0/2608
6	v	0.38	0/1938	0.43	0/2608
7	G	0.37	2/1929 (0.1%)	0.44	0/2607
7	U	0.37	1/1929 (0.1%)	0.44	0/2607
7	i	0.37	0/1929	0.44	0/2607
7	w	0.37	1/1929 (0.1%)	0.45	0/2607
8	H	0.31	0/1683	0.44	0/2276
8	V	0.31	0/1683	0.45	0/2276
8	j	0.31	0/1683	0.44	0/2276
8	x	0.31	0/1683	0.45	0/2276
9	I	0.34	0/1621	0.46	0/2185
9	W	0.33	1/1621 (0.1%)	0.45	0/2185



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	k	0.34	0/1621	0.45	0/2185
9	y	0.34	0/1621	0.45	0/2185
10	J	0.33	0/1602	0.45	0/2167
10	X	0.33	0/1602	0.45	0/2167
10	l	0.33	0/1602	0.45	0/2167
10	z	0.33	0/1602	0.46	0/2167
11	l	0.41	0/1588	0.44	0/2145
11	K	0.41	0/1588	0.44	0/2145
11	Y	0.41	0/1588	0.44	0/2145
11	m	0.41	0/1588	0.44	0/2145
12	2	0.32	0/1685	0.44	0/2271
12	L	0.32	0/1685	0.44	0/2271
12	Z	0.32	0/1685	0.44	0/2271
12	n	0.32	0/1685	0.43	0/2271
13	3	0.40	2/1718 (0.1%)	0.45	0/2325
13	M	0.40	1/1718 (0.1%)	0.46	0/2325
13	a	0.40	0/1718	0.45	0/2325
13	o	0.40	0/1718	0.45	0/2325
14	4	0.35	0/1546	0.42	0/2094
14	N	0.35	1/1546 (0.1%)	0.43	0/2094
14	b	0.35	0/1546	0.42	0/2094
14	p	0.35	0/1546	0.43	0/2094
All	All	0.36	17/99064 (0.0%)	0.45	0/133792

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	TRP	CD2-CE2	5.09	1.47	1.41
13	3	91	TRP	CD2-CE2	5.04	1.47	1.41
6	F	161	TRP	CD2-CE2	5.04	1.47	1.41
13	M	209	TRP	CD2-CE2	5.03	1.47	1.41
9	W	153	TRP	CD2-CE2	5.02	1.47	1.41
1	q	138	TRP	CD2-CE2	5.02	1.47	1.41
7	G	189	TRP	CD2-CE2	5.02	1.47	1.41
7	w	189	TRP	CD2-CE2	5.02	1.47	1.41
14	N	103	TRP	CD2-CE2	5.01	1.47	1.41
7	G	101	TRP	CD2-CE2	5.01	1.47	1.41
3	e	156	TRP	CD2-CE2	5.01	1.47	1.41
1	O	138	TRP	CD2-CE2	5.01	1.47	1.41
2	r	159	TRP	CD2-CE2	5.01	1.47	1.41
5	E	13	TRP	CD2-CE2	5.00	1.47	1.41
2	d	139	TRP	CD2-CE2	5.00	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	189	TRP	CD2-CE2	5.00	1.47	1.41
13	3	107	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	9	42
1	O	231/234 (99%)	217 (94%)	11 (5%)	3 (1%)	12	47
1	c	231/234 (99%)	213 (92%)	14 (6%)	4 (2%)	9	42
1	q	231/234 (99%)	213 (92%)	12 (5%)	6 (3%)	5	31
2	B	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	34	69
2	P	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	34	69
2	d	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	34	69
2	r	246/261 (94%)	239 (97%)	6 (2%)	1 (0%)	34	69
3	C	237/248 (96%)	226 (95%)	10 (4%)	1 (0%)	34	69
3	Q	237/248 (96%)	229 (97%)	7 (3%)	1 (0%)	34	69
3	e	237/248 (96%)	227 (96%)	8 (3%)	2 (1%)	19	58
3	s	237/248 (96%)	230 (97%)	6 (2%)	1 (0%)	34	69
4	D	231/241 (96%)	219 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	34	69
5	S	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
5	g	236/263 (90%)	227 (96%)	8 (3%)	1 (0%)	34	69
5	u	236/263 (90%)	224 (95%)	11 (5%)	1 (0%)	34	69
6	F	242/255 (95%)	229 (95%)	11 (4%)	2 (1%)	19	58
6	T	242/255 (95%)	228 (94%)	12 (5%)	2 (1%)	19	58
6	h	242/255 (95%)	230 (95%)	10 (4%)	2 (1%)	19	58
6	v	242/255 (95%)	229 (95%)	12 (5%)	1 (0%)	34	69
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%)	34	69
7	w	242/246 (98%)	232 (96%)	9 (4%)	1 (0%)	34	69
8	H	218/234 (93%)	204 (94%)	13 (6%)	1 (0%)	29	67
8	V	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	29	67
8	j	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	29	67
8	x	218/234 (93%)	204 (94%)	13 (6%)	1 (0%)	29	67
9	I	202/205 (98%)	187 (93%)	8 (4%)	7 (4%)	3	24
9	W	202/205 (98%)	189 (94%)	9 (4%)	4 (2%)	7	38
9	k	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	10	44
9	y	202/205 (98%)	186 (92%)	13 (6%)	3 (2%)	10	44
10	J	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	29	67
10	X	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	29	67
10	l	194/201 (96%)	182 (94%)	11 (6%)	1 (0%)	29	67
10	z	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	29	67
11	l	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	2	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	29	67
12	L	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	29	67
12	Z	211/213 (99%)	203 (96%)	7 (3%)	1 (0%)	29	67
12	n	211/213 (99%)	201 (95%)	9 (4%)	1 (0%)	29	67
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
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%)	29	67
All	All	12412/12920 (96%)	11795 (95%)	549 (4%)	68 (0%)	29	67

All (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
1	c	201	GLN
10	z	24	ASN
1	A	199	GLU
6	F	216	VAL
9	I	47	ARG
1	O	54	ILE
1	O	231	ALA
6	T	216	VAL
1	c	54	ILE
6	h	216	VAL
10	l	24	ASN
1	q	230	ALA
1	q	231	ALA
6	v	216	VAL
9	y	100	GLY
9	I	30	GLN

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Mol	Chain	Res	Type
9	I	46	ASP
3	Q	201	SER
9	W	30	GLN
1	c	199	GLU
3	e	201	SER
6	h	207	LYS
7	i	3	ARG
9	k	30	GLN
12	n	191	ASP
1	q	201	GLN
3	s	201	SER
7	w	3	ARG
9	y	30	GLN
9	y	155	PRO
12	2	191	ASP
1	A	231	ALA
8	H	188	PRO
9	I	16	LYS
12	L	191	ASP
2	P	206	LEU
9	W	45	GLY
12	Z	191	ASP
1	c	229	LEU
3	e	52	LYS
14	p	190	LEU
1	q	199	GLU
2	r	206	LEU
2	B	206	LEU
6	F	207	LYS
9	I	155	PRO
8	V	188	PRO
2	d	206	LEU
8	j	188	PRO
1	q	52	LYS
5	u	240	PRO
3	C	201	SER
6	T	3	ILE
1	q	54	ILE
8	x	188	PRO
9	W	100	GLY
5	g	240	PRO
5	E	240	PRO

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Mol	Chain	Res	Type
9	W	155	PRO
9	k	155	PRO
1	A	54	ILE
9	I	100	GLY
9	k	100	GLY

### 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	189/191 (99%)	185 (98%)	4 (2%)	53	79
1	O	189/191 (99%)	183 (97%)	6 (3%)	39	71
1	c	189/191 (99%)	181 (96%)	8 (4%)	30	65
1	q	189/191 (99%)	182 (96%)	7 (4%)	34	68
2	B	208/221 (94%)	200 (96%)	8 (4%)	33	67
2	P	208/221 (94%)	201 (97%)	7 (3%)	37	70
2	d	208/221 (94%)	202 (97%)	6 (3%)	42	74
2	r	208/221 (94%)	195 (94%)	13 (6%)	18	52
3	C	202/211 (96%)	192 (95%)	10 (5%)	24	60
3	Q	202/211 (96%)	193 (96%)	9 (4%)	27	63
3	e	202/211 (96%)	194 (96%)	8 (4%)	31	66
3	s	202/211 (96%)	193 (96%)	9 (4%)	27	63
4	D	195/203 (96%)	189 (97%)	6 (3%)	40	72
4	R	195/203 (96%)	192 (98%)	3 (2%)	65	85
4	f	195/203 (96%)	192 (98%)	3 (2%)	65	85
4	t	195/203 (96%)	191 (98%)	4 (2%)	53	79
5	E	204/224 (91%)	198 (97%)	6 (3%)	42	74
5	S	204/224 (91%)	194 (95%)	10 (5%)	25	61
5	g	204/224 (91%)	196 (96%)	8 (4%)	32	67
5	u	204/224 (91%)	196 (96%)	8 (4%)	32	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	200/211 (95%)	195 (98%)	5 (2%)	47	77
6	T	200/211 (95%)	194 (97%)	6 (3%)	41	73
6	h	200/211 (95%)	194 (97%)	6 (3%)	41	73
6	v	200/211 (95%)	194 (97%)	6 (3%)	41	73
7	G	207/210 (99%)	200 (97%)	7 (3%)	37	70
7	U	207/210 (99%)	199 (96%)	8 (4%)	32	67
7	i	207/210 (99%)	202 (98%)	5 (2%)	49	77
7	w	207/210 (99%)	196 (95%)	11 (5%)	22	58
8	H	181/195 (93%)	176 (97%)	5 (3%)	43	74
8	V	181/195 (93%)	179 (99%)	2 (1%)	73	88
8	j	181/195 (93%)	180 (99%)	1 (1%)	86	94
8	x	181/195 (93%)	177 (98%)	4 (2%)	52	79
9	I	174/175 (99%)	171 (98%)	3 (2%)	60	83
9	W	174/175 (99%)	171 (98%)	3 (2%)	60	83
9	k	174/175 (99%)	170 (98%)	4 (2%)	50	78
9	y	174/175 (99%)	170 (98%)	4 (2%)	50	78
10	J	166/171 (97%)	161 (97%)	5 (3%)	41	73
10	X	166/171 (97%)	163 (98%)	3 (2%)	59	82
10	l	166/171 (97%)	165 (99%)	1 (1%)	86	94
10	z	166/171 (97%)	159 (96%)	7 (4%)	30	65
11	1	157/161 (98%)	155 (99%)	2 (1%)	69	87
11	K	157/161 (98%)	154 (98%)	3 (2%)	57	81
11	Y	157/161 (98%)	154 (98%)	3 (2%)	57	81
11	m	157/161 (98%)	153 (98%)	4 (2%)	47	77
12	2	178/178 (100%)	171 (96%)	7 (4%)	32	67
12	L	178/178 (100%)	171 (96%)	7 (4%)	32	67
12	Z	178/178 (100%)	176 (99%)	2 (1%)	73	88
12	n	178/178 (100%)	171 (96%)	7 (4%)	32	67
13	3	178/180 (99%)	173 (97%)	5 (3%)	43	74
13	M	178/180 (99%)	175 (98%)	3 (2%)	60	83
13	a	178/180 (99%)	175 (98%)	3 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	o	178/180 (99%)	174 (98%)	4 (2%)	52	79
14	4	159/162 (98%)	159 (100%)	0	100	100
14	N	159/162 (98%)	157 (99%)	2 (1%)	69	87
14	b	159/162 (98%)	158 (99%)	1 (1%)	86	94
14	p	159/162 (98%)	156 (98%)	3 (2%)	57	81
All	All	10392/10772 (96%)	10097 (97%)	295 (3%)	43	74

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	194	LEU
1	A	207	ILE
1	A	214	GLU
2	B	25	MET
2	B	44	LEU
2	B	98	LEU
2	B	155	ASN
2	B	178	ASP
2	B	199	LYS
2	B	218	ARG
2	B	229	LYS
3	C	43	LEU
3	C	47	LYS
3	C	107	ILE
3	C	139	ASP
3	C	172	LEU
3	C	178	ASP
3	C	184	ASP
3	C	185	ASP
3	C	213	ARG
3	C	221	ASN
4	D	148	GLU
4	D	203	LYS
4	D	208	GLU
4	D	209	LYS
4	D	217	LEU
4	D	240	ASP
5	E	5	GLN
5	E	38	LEU

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Mol	Chain	Res	Type
5	E	74	ILE
5	E	101	ARG
5	E	187	LEU
5	E	209	ASN
6	F	56	LYS
6	F	129	ARG
6	F	181	MET
6	F	203	GLU
6	F	205	LYS
7	G	84	THR
7	G	86	ASP
7	G	131	MET
7	G	166	THR
7	G	209	ASP
7	G	210	PHE
7	G	221	THR
8	H	6	VAL
8	H	40	ASN
8	H	180	LYS
8	H	194	LYS
8	H	201	ARG
9	I	19	VAL
9	I	136	VAL
9	I	144	GLN
10	J	8	GLN
10	J	45	LEU
10	J	85	ARG
10	J	143	LEU
10	J	191	LEU
11	K	58	LEU
11	K	71	LYS
11	K	176	LEU
12	L	45	LYS
12	L	62	LEU
12	L	67	ILE
12	L	118	LYS
12	L	148	LEU
12	L	160	ASN
12	L	173	ARG
13	M	44	ARG
13	M	46	ASN
13	M	94	ARG

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Mol	Chain	Res	Type
14	N	116	MET
14	N	194	ILE
1	O	54	ILE
1	O	81	ASP
1	O	176	ARG
1	O	192	LEU
1	O	194	LEU
1	O	207	ILE
2	P	25	MET
2	P	37	ILE
2	P	44	LEU
2	P	56	LEU
2	P	98	LEU
2	P	178	ASP
2	P	218	ARG
3	Q	5	ARG
3	Q	43	LEU
3	Q	99	GLU
3	Q	107	ILE
3	Q	139	ASP
3	Q	172	LEU
3	Q	178	ASP
3	Q	221	ASN
3	Q	236	LYS
4	R	203	LYS
4	R	209	LYS
4	R	224	GLN
5	S	38	LEU
5	S	74	ILE
5	S	84	LEU
5	S	101	ARG
5	S	139	ASP
5	S	187	LEU
5	S	202	GLU
5	S	206	THR
5	S	209	ASN
5	S	211	SER
6	T	56	LYS
6	T	108	LEU
6	T	129	ARG
6	T	181	MET
6	T	187	ARG

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Mol	Chain	Res	Type
6	T	233	GLU
7	U	52	THR
7	U	131	MET
7	U	166	THR
7	U	179	LEU
7	U	186	LYS
7	U	209	ASP
7	U	221	THR
7	U	226	LYS
8	V	40	ASN
8	V	180	LYS
9	W	13	MET
9	W	136	VAL
9	W	144	GLN
10	X	143	LEU
10	X	154	GLU
10	X	191	LEU
11	Y	58	LEU
11	Y	71	LYS
11	Y	176	LEU
12	Z	160	ASN
12	Z	173	ARG
13	a	44	ARG
13	a	46	ASN
13	a	94	ARG
14	b	173	VAL
1	c	2	LYS
1	c	54	ILE
1	c	81	ASP
1	c	83	ARG
1	c	181	LEU
1	c	194	LEU
1	c	207	ILE
1	c	229	LEU
2	d	25	MET
2	d	44	LEU
2	d	98	LEU
2	d	164	ILE
2	d	198	ASN
2	d	199	LYS
3	e	5	ARG
3	e	52	LYS

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Mol	Chain	Res	Type
3	e	96	LEU
3	e	107	ILE
3	e	125	ARG
3	e	185	ASP
3	e	213	ARG
3	e	221	ASN
4	f	84	ASP
4	f	126	GLU
4	f	217	LEU
5	g	38	LEU
5	g	56	LEU
5	g	74	ILE
5	g	83	LEU
5	g	101	ARG
5	g	187	LEU
5	g	209	ASN
5	g	241	GLN
6	h	3	ILE
6	h	19	ARG
6	h	37	ILE
6	h	56	LYS
6	h	64	LYS
6	h	181	MET
7	i	86	ASP
7	i	166	THR
7	i	170	VAL
7	i	210	PHE
7	i	221	THR
8	j	40	ASN
9	k	16	LYS
9	k	136	VAL
9	k	144	GLN
9	k	192	ASP
10	l	8	GLN
11	m	32	LYS
11	m	58	LEU
11	m	97	MET
11	m	176	LEU
12	n	45	LYS
12	n	67	ILE
12	n	131	GLN
12	n	148	LEU

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Mol	Chain	Res	Type
12	n	160	ASN
12	n	166	LEU
12	n	173	ARG
13	o	44	ARG
13	o	46	ASN
13	o	94	ARG
13	o	159	VAL
14	p	95	MET
14	p	122	ARG
14	p	173	VAL
1	q	51	GLN
1	q	81	ASP
1	q	83	ARG
1	q	205	ASP
1	q	207	ILE
1	q	214	GLU
1	q	218	ARG
2	r	25	MET
2	r	44	LEU
2	r	50	ARG
2	r	164	ILE
2	r	178	ASP
2	r	199	LYS
2	r	201	MET
2	r	218	ARG
2	r	222	LYS
2	r	236	LEU
2	r	242	GLU
2	r	243	GLU
2	r	248	GLU
3	s	39	ASP
3	s	96	LEU
3	s	99	GLU
3	s	107	ILE
3	s	139	ASP
3	s	185	ASP
3	s	213	ARG
3	s	221	ASN
3	s	225	ILE
4	t	203	LYS
4	t	209	LYS
4	t	217	LEU

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Mol	Chain	Res	Type
4	t	240	ASP
5	u	38	LEU
5	u	39	LYS
5	u	56	LEU
5	u	74	ILE
5	u	101	ARG
5	u	126	ARG
5	u	205	LEU
5	u	241	GLN
6	v	56	LYS
6	v	129	ARG
6	v	170	GLN
6	v	181	MET
6	v	203	GLU
6	v	232	ARG
7	w	56	VAL
7	w	60	LEU
7	w	86	ASP
7	w	92	GLN
7	w	131	MET
7	w	166	THR
7	w	179	LEU
7	w	182	LYS
7	w	209	ASP
7	w	210	PHE
7	w	221	THR
8	x	9	LYS
8	x	58	LEU
8	x	180	LYS
8	x	201	ARG
9	y	33	MET
9	y	136	VAL
9	y	144	GLN
9	y	171	LEU
10	z	8	GLN
10	z	45	LEU
10	z	103	LEU
10	z	143	LEU
10	z	154	GLU
10	z	155	ARG
10	z	191	LEU
11	1	58	LEU

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Mol	Chain	Res	Type
11	1	71	LYS
12	2	62	LEU
12	2	67	ILE
12	2	127	VAL
12	2	148	LEU
12	2	160	ASN
12	2	166	LEU
12	2	173	ARG
13	3	35	ARG
13	3	44	ARG
13	3	46	ASN
13	3	69	GLN
13	3	94	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	206	ASN
2	B	123	GLN
2	B	155	ASN
3	C	23	GLN
3	C	221	ASN
4	D	152	GLN
4	D	186	HIS
5	E	5	GLN
5	E	60	GLN
5	E	146	GLN
5	E	209	ASN
7	G	92	GLN
7	G	127	GLN
8	H	40	ASN
9	I	6	ASN
9	I	64	GLN
9	I	144	GLN
10	J	8	GLN
10	J	61	GLN
10	J	82	ASN
11	K	38	ASN
12	L	8	ASN
12	L	131	GLN
13	M	46	ASN

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Mol	Chain	Res	Type
13	M	157	GLN
14	N	123	GLN
1	O	139	ASN
1	O	206	ASN
2	P	88	ASN
2	P	95	GLN
2	P	109	GLN
2	P	123	GLN
2	P	155	ASN
3	Q	23	GLN
3	Q	221	ASN
4	R	186	HIS
4	R	224	GLN
5	S	60	GLN
5	S	146	GLN
5	S	209	ASN
6	T	147	GLN
7	U	92	GLN
7	U	127	GLN
8	V	40	ASN
8	V	66	HIS
8	V	116	HIS
9	W	6	ASN
9	W	39	GLN
9	W	64	GLN
9	W	144	GLN
10	X	82	ASN
11	Y	38	ASN
12	Z	8	ASN
12	Z	77	HIS
12	Z	108	ASN
12	Z	131	GLN
12	Z	146	GLN
13	a	46	ASN
1	c	94	GLN
1	c	139	ASN
1	c	206	ASN
2	d	95	GLN
2	d	109	GLN
2	d	123	GLN
2	d	155	ASN
3	e	221	ASN

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Mol	Chain	Res	Type
4	f	204	GLN
5	g	146	GLN
5	g	209	ASN
7	i	92	GLN
7	i	127	GLN
8	j	40	ASN
9	k	6	ASN
9	k	64	GLN
9	k	144	GLN
9	k	161	HIS
10	l	8	GLN
10	l	61	GLN
11	m	29	GLN
11	m	38	ASN
12	n	8	ASN
12	n	131	GLN
12	n	146	GLN
13	o	46	ASN
13	o	81	HIS
13	o	147	GLN
13	o	157	GLN
14	p	7	GLN
14	p	123	GLN
1	q	51	GLN
1	q	139	ASN
1	q	206	ASN
2	r	88	ASN
2	r	95	GLN
2	r	109	GLN
2	r	123	GLN
3	s	23	GLN
3	s	221	ASN
4	t	114	GLN
4	t	204	GLN
4	t	211	ASN
5	u	60	GLN
5	u	146	GLN
5	u	209	ASN
7	w	92	GLN
7	w	127	GLN
8	x	40	ASN
9	y	6	ASN

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Mol	Chain	Res	Type
9	y	144	GLN
10	z	8	GLN
10	z	132	HIS
11	1	29	GLN
11	1	38	ASN
12	2	8	ASN
12	2	146	GLN
13	3	2	GLN
13	3	46	ASN
13	3	69	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 monosaccharides 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	-0.01	3 (1%) 77 65	68, 101, 151, 178	0
1	O	233/234 (99%)	-0.12	4 (1%) 70 57	56, 79, 133, 166	0
1	c	233/234 (99%)	-0.02	2 (0%) 84 75	75, 107, 157, 181	0
1	q	233/234 (99%)	-0.05	3 (1%) 77 65	80, 107, 155, 173	0
2	B	248/261 (95%)	-0.11	2 (0%) 86 78	65, 95, 143, 169	0
2	P	248/261 (95%)	-0.21	3 (1%) 79 67	51, 78, 117, 157	0
2	d	248/261 (95%)	0.14	14 (5%) 24 13	65, 110, 164, 202	0
2	r	248/261 (95%)	-0.07	2 (0%) 86 78	78, 110, 148, 167	0
3	C	239/248 (96%)	0.17	6 (2%) 57 43	73, 109, 169, 202	0
3	Q	239/248 (96%)	0.08	4 (1%) 70 57	61, 98, 156, 197	0
3	e	239/248 (96%)	0.39	16 (6%) 17 10	80, 125, 178, 204	0
3	s	239/248 (96%)	0.23	11 (4%) 32 20	91, 125, 174, 196	0
4	D	233/241 (96%)	-0.16	0 100 100	59, 96, 130, 154	0
4	R	233/241 (96%)	-0.14	4 (1%) 70 57	67, 101, 139, 176	0
4	f	233/241 (96%)	-0.03	3 (1%) 77 65	77, 124, 155, 185	0
4	t	233/241 (96%)	-0.01	1 (0%) 92 89	71, 120, 157, 190	0
5	E	238/263 (90%)	-0.14	2 (0%) 86 78	57, 93, 148, 178	0
5	S	238/263 (90%)	0.04	4 (1%) 70 57	66, 98, 154, 184	0
5	g	238/263 (90%)	0.09	1 (0%) 92 89	81, 117, 163, 192	0
5	u	238/263 (90%)	0.04	3 (1%) 77 65	66, 108, 162, 182	0
6	F	244/255 (95%)	0.03	3 (1%) 79 67	63, 97, 146, 162	0
6	T	244/255 (95%)	-0.04	5 (2%) 65 51	58, 89, 143, 168	0
6	h	244/255 (95%)	0.13	3 (1%) 79 67	87, 121, 165, 179	0
6	v	244/255 (95%)	-0.02	1 (0%) 92 89	81, 109, 149, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	G	244/246 (99%)	0.02	4 (1%) 72 59	66, 101, 149, 170	0
7	U	244/246 (99%)	-0.20	1 (0%) 92 89	57, 81, 114, 144	0
7	i	244/246 (99%)	0.16	9 (3%) 41 26	81, 121, 159, 180	0
7	w	244/246 (99%)	-0.01	2 (0%) 86 78	78, 107, 150, 169	0
8	H	220/234 (94%)	-0.09	1 (0%) 91 86	62, 81, 130, 169	0
8	V	220/234 (94%)	-0.23	0 100 100	49, 65, 103, 153	0
8	j	220/234 (94%)	-0.11	1 (0%) 91 86	71, 87, 125, 151	0
8	x	220/234 (94%)	-0.09	1 (0%) 91 86	69, 93, 142, 175	0
9	I	204/205 (99%)	-0.18	0 100 100	64, 79, 118, 146	0
9	W	204/205 (99%)	-0.30	0 100 100	52, 66, 96, 129	0
9	k	204/205 (99%)	-0.21	0 100 100	69, 84, 120, 141	0
9	y	204/205 (99%)	-0.11	1 (0%) 91 86	75, 100, 146, 156	0
10	J	196/201 (97%)	-0.23	0 100 100	58, 75, 104, 124	0
10	X	196/201 (97%)	-0.33	0 100 100	53, 70, 99, 132	0
10	l	196/201 (97%)	-0.19	1 (0%) 91 86	66, 92, 122, 146	0
10	z	196/201 (97%)	-0.26	0 100 100	70, 95, 130, 158	0
11	1	201/205 (98%)	-0.16	1 (0%) 91 86	60, 86, 119, 147	0
11	K	201/205 (98%)	-0.31	0 100 100	53, 70, 102, 123	0
11	Y	201/205 (98%)	-0.22	0 100 100	59, 77, 106, 137	0
11	m	201/205 (98%)	-0.23	0 100 100	69, 95, 130, 159	0
12	2	213/213 (100%)	-0.18	0 100 100	66, 84, 110, 157	0
12	L	213/213 (100%)	-0.23	1 (0%) 91 86	53, 68, 98, 146	0
12	Z	213/213 (100%)	-0.12	0 100 100	56, 84, 125, 173	0
12	n	213/213 (100%)	-0.05	1 (0%) 91 86	75, 102, 138, 166	0
13	3	216/219 (98%)	-0.14	3 (1%) 75 63	65, 82, 112, 153	0
13	M	216/219 (98%)	-0.22	0 100 100	54, 70, 99, 119	0
13	a	216/219 (98%)	-0.20	0 100 100	53, 75, 106, 129	0
13	o	216/219 (98%)	-0.15	0 100 100	64, 91, 122, 132	0
14	4	202/205 (98%)	-0.03	4 (1%) 65 51	61, 86, 125, 159	0
14	N	202/205 (98%)	-0.12	3 (1%) 73 61	47, 74, 112, 157	0
14	b	202/205 (98%)	-0.11	3 (1%) 73 61	55, 69, 113, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	p	202/205 (98%)	0.01	3 (1%) 73 61	68, 89, 139, 164	0
All	All	12524/12920 (96%)	-0.08	140 (1%) 80 69	47, 93, 150, 204	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	233	ALA	10.0
1	A	233	ALA	8.8
6	F	1	SER	6.9
14	b	201	THR	6.6
2	d	247	ALA	6.6
6	T	1	SER	6.5
6	v	1	SER	5.9
6	h	1	SER	5.5
1	c	233	ALA	5.4
6	T	2	SER	5.1
2	d	245	ALA	4.8
6	T	3	ILE	4.7
14	4	202	LEU	4.7
8	x	199	LEU	4.6
2	d	249	ARG	4.3
4	f	241	ILE	4.1
3	s	220	LEU	4.0
4	t	241	ILE	4.0
3	Q	240	GLU	3.9
6	F	2	SER	3.8
14	b	200	ALA	3.7
2	d	246	LYS	3.6
2	d	209	GLU	3.6
2	d	244	GLU	3.4
4	R	241	ILE	3.4
3	s	238	GLU	3.3
7	i	212	PRO	3.3
1	O	232	ILE	3.2
1	q	1	ALA	3.2
5	u	240	PRO	3.1
14	4	201	THR	3.1
3	e	47	LYS	3.1
2	d	205	LYS	3.1
14	p	201	THR	3.0
3	C	38	LYS	3.0
10	l	158	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
5	S	158	ALA	3.0
3	e	239	ASN	2.9
1	q	233	ALA	2.9
3	C	179	ASP	2.9
5	u	218	ASP	2.9
8	H	199	LEU	2.8
7	i	3	ARG	2.8
1	O	199	GLU	2.8
2	d	248	GLU	2.8
14	p	153	LEU	2.8
7	i	181	LYS	2.8
14	p	200	ALA	2.8
3	e	43	LEU	2.8
7	G	2	SER	2.7
5	E	240	PRO	2.7
3	e	40	ILE	2.7
7	G	242	LEU	2.7
3	s	180	ALA	2.7
7	U	59	LYS	2.7
2	r	202	ASP	2.7
5	g	240	PRO	2.7
2	d	204	SER	2.6
2	P	202	ASP	2.6
1	A	1	ALA	2.6
3	s	40	ILE	2.6
2	d	178	ASP	2.6
3	e	179	ASP	2.6
12	n	1	ARG	2.6
2	P	205	LYS	2.5
14	4	198	THR	2.5
3	s	207	GLU	2.5
6	T	5	THR	2.5
4	f	44	GLU	2.5
3	e	206	ILE	2.5
3	e	38	LYS	2.5
4	f	45	GLY	2.5
14	N	201	THR	2.5
2	d	242	GLU	2.5
3	e	204	LYS	2.5
3	s	237	GLU	2.4
5	E	204	ASP	2.4
2	d	243	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
14	4	199	ILE	2.4
6	T	215	TRP	2.4
4	R	200	ILE	2.4
14	b	202	LEU	2.4
6	h	3	ILE	2.4
1	c	170	LYS	2.4
3	e	183	THR	2.4
3	s	35	VAL	2.4
3	s	206	ILE	2.4
3	C	204	LYS	2.4
2	r	205	LYS	2.4
1	A	227	ASP	2.3
13	3	167	GLU	2.3
7	i	202	LEU	2.3
1	q	3	ARG	2.3
4	R	239	LYS	2.3
6	F	244	LYS	2.3
6	h	60	GLU	2.3
3	e	202	GLY	2.3
2	d	231	LYS	2.3
3	s	172	LEU	2.3
7	G	191	PHE	2.3
3	e	238	GLU	2.3
3	e	200	GLN	2.3
3	e	236	LYS	2.3
5	S	229	VAL	2.3
3	C	35	VAL	2.2
3	Q	47	LYS	2.2
3	e	203	GLY	2.2
7	i	52	THR	2.2
2	P	204	SER	2.2
8	j	199	LEU	2.2
12	L	162	GLU	2.2
7	i	210	PHE	2.2
7	i	241	ALA	2.2
7	w	212	PRO	2.2
13	3	114	GLY	2.2
3	e	158	ALA	2.1
7	i	239	LEU	2.1
3	Q	239	ASN	2.1
3	C	237	GLU	2.1
3	Q	179	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	R	196	LYS	2.1
9	y	114	LYS	2.1
7	i	208	ILE	2.1
14	N	199	ILE	2.1
5	u	56	LEU	2.1
14	N	198	THR	2.1
3	C	203	GLY	2.1
3	e	139	ASP	2.0
11	l	181	GLU	2.0
3	s	204	LYS	2.0
3	s	234	LYS	2.0
5	S	176	MET	2.0
13	3	119	GLU	2.0
2	B	206	LEU	2.0
2	B	187	LYS	2.0
7	G	188	ASP	2.0
2	d	213	ILE	2.0
1	O	2	LYS	2.0
5	S	241	GLN	2.0
7	w	186	LYS	2.0

## 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 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.