



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:25 AM GMT

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 wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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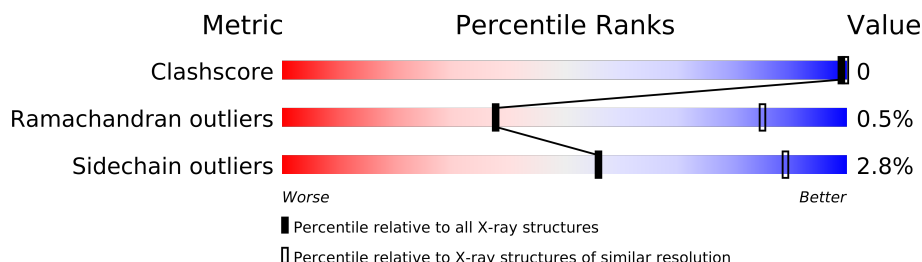
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	<b>FAILED</b>
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.










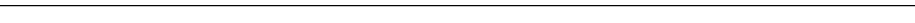
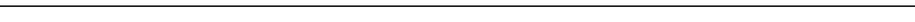
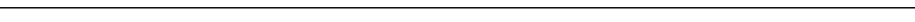


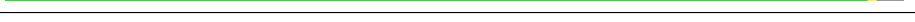


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	234	
1	O	234	
1	c	234	
1	q	234	
2	B	261	
2	P	261	
2	d	261	
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	

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

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 97956 atoms, of which 0 are hydrogen and 0 are deuterium.

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

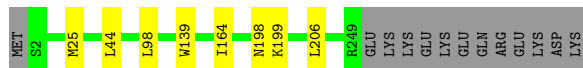
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	n	13	Total 13	O 13	0	0
15	o	11	Total 11	O 11	0	0
15	p	6	Total 6	O 6	0	0
15	q	3	Total 3	O 3	0	0
15	r	10	Total 10	O 10	0	0
15	s	7	Total 7	O 7	0	0
15	t	6	Total 6	O 6	0	0
15	u	7	Total 7	O 7	0	0
15	v	11	Total 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



- Chain d: 



- Chain r:



- Chain C: 



- Chain Q: 



- Chain e: 



- Chain s: 



- Chain D: 

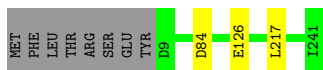


- Chain R: 



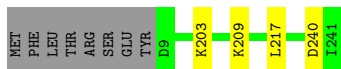
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Chain f: 



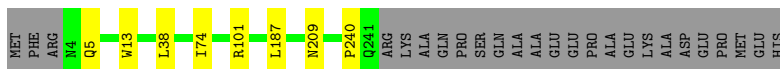
- Molecule 4: Proteasome subunit alpha type-5

Chain t: 



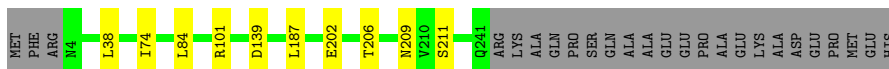
- Molecule 5: Proteasome subunit alpha type-1

Chain E: 



- Molecule 5: Proteasome subunit alpha type-1

Chain S: 



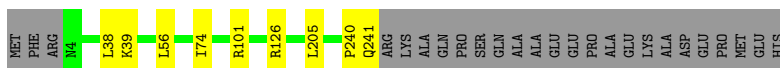
- Molecule 5: Proteasome subunit alpha type-1

Chain g: 



- Molecule 5: Proteasome subunit alpha type-1

Chain u: 



- Molecule 6: Proteasome subunit alpha type-3

Chain F: 



- Molecule 6: Proteasome subunit alpha type-3

Chain T: 



- Molecule 6: Proteasome subunit alpha type-3

Chain h: 



- Molecule 6: Proteasome subunit alpha type-3

Chain v:



- Molecule 7: Proteasome subunit alpha type-6

Chain G:



- Molecule 7: Proteasome subunit alpha type-6

Chain U:



- Molecule 7: Proteasome subunit alpha type-6

Chain i:



- Molecule 7: Proteasome subunit alpha type-6

Chain w:



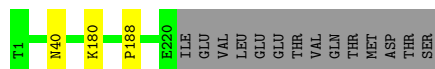
- Molecule 8: Proteasome subunit beta type-7

Chain H:



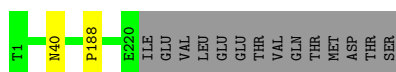
- Molecule 8: Proteasome subunit beta type-7

Chain V:



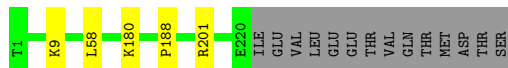
- Molecule 8: Proteasome subunit beta type-7

Chain j:



- Molecule 8: Proteasome subunit beta type-7

Chain x:



- Molecule 9: Proteasome subunit beta type-3

Chain I:



- Molecule 9: Proteasome subunit beta type-3

Chain W:



- Molecule 9: Proteasome subunit beta type-3

Chain k:



- Molecule 9: Proteasome subunit beta type-3

Chain y:



- Molecule 10: Proteasome subunit beta type-2

Chain J:



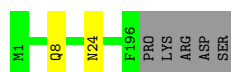
- Molecule 10: Proteasome subunit beta type-2

Chain X:



- Molecule 10: Proteasome subunit beta type-2

Chain l:



- Molecule 10: Proteasome subunit beta type-2

Chain z:



- Molecule 11: Proteasome subunit beta type-5

Chain K:



- Molecule 11: Proteasome subunit beta type-5

Chain Y:



- Molecule 11: Proteasome subunit beta type-5

Chain m:



- Molecule 11: Proteasome subunit beta type-5

Chain 1:



- Molecule 12: Proteasome subunit beta type-1

Chain L:



- Molecule 12: Proteasome subunit beta type-1

Chain Z:



- Molecule 12: Proteasome subunit beta type-1

Chain n:





- Molecule 12: Proteasome subunit beta type-1

Chain 2:



- Molecule 13: Proteasome subunit beta type-4

Chain M:



- Molecule 13: Proteasome subunit beta type-4

Chain a:



- Molecule 13: Proteasome subunit beta type-4

Chain o:



- Molecule 13: Proteasome subunit beta type-4

Chain 3:



- Molecule 14: Proteasome subunit beta type-6

Chain N:



- Molecule 14: Proteasome subunit beta type-6

Chain b:



- Molecule 14: Proteasome subunit beta type-6

Chain p:



- Molecule 14: Proteasome subunit beta type-6

Chain 4: 



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	98.1 (15.00-3.20)	Depositor
$R_{merge}$	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	Depositor
Wilson B-factor (Å <sup>2</sup> )	84.9	Xtriage
Anisotropy	0.316	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	6 of 235050 reflections (0.003%)	Xtriage
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.

## 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

The worst 5 of 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

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1817	0	0	1	0
1	O	1817	0	0	1	0
1	c	1817	0	0	0	0
1	q	1817	0	0	0	0
2	B	1950	0	0	0	0
2	P	1950	0	0	0	0
2	d	1950	0	0	0	0
2	r	1950	0	0	0	0
3	C	1881	0	0	0	0
3	Q	1881	0	0	0	0
3	e	1881	0	0	0	0
3	s	1881	0	0	0	0
4	D	1778	0	0	0	0
4	R	1778	0	0	0	0
4	f	1778	0	0	0	0
4	t	1778	0	0	0	0
5	E	1872	0	0	0	0
5	S	1872	0	0	0	0
5	g	1872	0	0	0	0
5	u	1872	0	0	0	0
6	F	1903	0	0	0	0
6	T	1903	0	0	0	0
6	h	1903	0	0	0	0
6	v	1903	0	0	0	0
7	G	1895	0	0	0	0
7	U	1895	0	0	0	0
7	i	1895	0	0	0	0
7	w	1895	0	0	0	0
8	H	1656	0	0	0	0
8	V	1656	0	0	0	0
8	j	1656	0	0	0	0
8	x	1656	0	0	0	0
9	I	1592	0	0	2	0
9	W	1592	0	0	0	0
9	k	1592	0	0	0	0
9	y	1592	0	0	0	0
10	J	1570	0	0	0	0
10	X	1570	0	0	0	0
10	l	1570	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	z	1570	0	0	0	0
11	1	1557	0	0	0	0
11	K	1557	0	0	1	0
11	Y	1557	0	0	1	0
11	m	1557	0	0	0	0
12	2	1654	0	0	0	0
12	L	1654	0	0	0	0
12	Z	1654	0	0	0	0
12	n	1654	0	0	0	0
13	3	1685	0	0	0	0
13	M	1685	0	0	0	0
13	a	1685	0	0	0	0
13	o	1685	0	0	0	0
14	4	1519	0	0	0	0
14	N	1519	0	0	1	0
14	b	1519	0	0	0	0
14	p	1519	0	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	0	7	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

The worst 5 of 7 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:30:VAL:CG1	14:N:30:VAL:O	2.56	0.53
9:I:115:THR:O	9:I:117:LYS:N	2.45	0.50
9:I:46:ASP:O	9:I:47:ARG:CB	2.59	0.49
11:K:38:ASN:O	11:K:184:TRP:NE1	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:230:ALA:O	1:O:232:ILE:N	2.51	0.44

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	14	62
1	O	231/234 (99%)	217 (94%)	11 (5%)	3 (1%)	18	68
1	c	231/234 (99%)	213 (92%)	14 (6%)	4 (2%)	14	62
1	q	231/234 (99%)	213 (92%)	12 (5%)	6 (3%)	8	47
2	B	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	43	88
2	P	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	43	88
2	d	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	43	88
2	r	246/261 (94%)	239 (97%)	6 (2%)	1 (0%)	43	88
3	C	237/248 (96%)	226 (95%)	10 (4%)	1 (0%)	43	88
3	Q	237/248 (96%)	229 (97%)	7 (3%)	1 (0%)	43	88
3	e	237/248 (96%)	227 (96%)	8 (3%)	2 (1%)	27	77
3	s	237/248 (96%)	230 (97%)	6 (2%)	1 (0%)	43	88
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%)	43	88
5	S	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
5	g	236/263 (90%)	227 (96%)	8 (3%)	1 (0%)	43	88
5	u	236/263 (90%)	224 (95%)	11 (5%)	1 (0%)	43	88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	242/255 (95%)	229 (95%)	11 (4%)	2 (1%)	27	77
6	T	242/255 (95%)	228 (94%)	12 (5%)	2 (1%)	27	77
6	h	242/255 (95%)	230 (95%)	10 (4%)	2 (1%)	27	77
6	v	242/255 (95%)	229 (95%)	12 (5%)	1 (0%)	43	88
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%)	43	88
7	w	242/246 (98%)	232 (96%)	9 (4%)	1 (0%)	43	88
8	H	218/234 (93%)	204 (94%)	13 (6%)	1 (0%)	38	85
8	V	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	38	85
8	j	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	38	85
8	x	218/234 (93%)	204 (94%)	13 (6%)	1 (0%)	38	85
9	I	202/205 (98%)	187 (93%)	8 (4%)	7 (4%)	6	37
9	W	202/205 (98%)	189 (94%)	9 (4%)	4 (2%)	11	56
9	k	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	15	64
9	y	202/205 (98%)	186 (92%)	13 (6%)	3 (2%)	15	64
10	J	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	38	85
10	X	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	38	85
10	l	194/201 (96%)	182 (94%)	11 (6%)	1 (0%)	38	85
10	z	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	38	85
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%)	38	85
12	L	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	38	85
12	Z	211/213 (99%)	203 (96%)	7 (3%)	1 (0%)	38	85
12	n	211/213 (99%)	201 (95%)	9 (4%)	1 (0%)	38	85
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	38	85
All	All	12412/12920 (96%)	11795 (95%)	549 (4%)	68 (0%)	38	85

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 ⓘ

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%)	66	92
1	O	189/191 (99%)	183 (97%)	6 (3%)	51	87
1	c	189/191 (99%)	181 (96%)	8 (4%)	40	82
1	q	189/191 (99%)	182 (96%)	7 (4%)	45	85
2	B	208/221 (94%)	200 (96%)	8 (4%)	44	84
2	P	208/221 (94%)	201 (97%)	7 (3%)	49	86
2	d	208/221 (94%)	202 (97%)	6 (3%)	55	88
2	r	208/221 (94%)	195 (94%)	13 (6%)	25	69
3	C	202/211 (96%)	192 (95%)	10 (5%)	34	78
3	Q	202/211 (96%)	193 (96%)	9 (4%)	38	81
3	e	202/211 (96%)	194 (96%)	8 (4%)	42	83
3	s	202/211 (96%)	193 (96%)	9 (4%)	38	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	195/203 (96%)	189 (97%)	6 (3%)	52	88
4	R	195/203 (96%)	192 (98%)	3 (2%)	76	95
4	f	195/203 (96%)	192 (98%)	3 (2%)	76	95
4	t	195/203 (96%)	191 (98%)	4 (2%)	66	92
5	E	204/224 (91%)	198 (97%)	6 (3%)	55	88
5	S	204/224 (91%)	194 (95%)	10 (5%)	35	79
5	g	204/224 (91%)	196 (96%)	8 (4%)	43	84
5	u	204/224 (91%)	196 (96%)	8 (4%)	43	84
6	F	200/211 (95%)	195 (98%)	5 (2%)	60	90
6	T	200/211 (95%)	194 (97%)	6 (3%)	53	88
6	h	200/211 (95%)	194 (97%)	6 (3%)	53	88
6	v	200/211 (95%)	194 (97%)	6 (3%)	53	88
7	G	207/210 (99%)	200 (97%)	7 (3%)	49	86
7	U	207/210 (99%)	199 (96%)	8 (4%)	43	84
7	i	207/210 (99%)	202 (98%)	5 (2%)	61	91
7	w	207/210 (99%)	196 (95%)	11 (5%)	32	75
8	H	181/195 (93%)	176 (97%)	5 (3%)	56	89
8	V	181/195 (93%)	179 (99%)	2 (1%)	84	96
8	j	181/195 (93%)	180 (99%)	1 (1%)	92	98
8	x	181/195 (93%)	177 (98%)	4 (2%)	64	91
9	I	174/175 (99%)	171 (98%)	3 (2%)	73	94
9	W	174/175 (99%)	171 (98%)	3 (2%)	73	94
9	k	174/175 (99%)	170 (98%)	4 (2%)	63	91
9	y	174/175 (99%)	170 (98%)	4 (2%)	63	91
10	J	166/171 (97%)	161 (97%)	5 (3%)	53	88
10	X	166/171 (97%)	163 (98%)	3 (2%)	71	93
10	l	166/171 (97%)	165 (99%)	1 (1%)	92	98
10	z	166/171 (97%)	159 (96%)	7 (4%)	40	82
11	l	157/161 (98%)	155 (99%)	2 (1%)	80	95
11	K	157/161 (98%)	154 (98%)	3 (2%)	69	93
11	Y	157/161 (98%)	154 (98%)	3 (2%)	69	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	m	157/161 (98%)	153 (98%)	4 (2%)	60	90
12	2	178/178 (100%)	171 (96%)	7 (4%)	43	84
12	L	178/178 (100%)	171 (96%)	7 (4%)	43	84
12	Z	178/178 (100%)	176 (99%)	2 (1%)	84	96
12	n	178/178 (100%)	171 (96%)	7 (4%)	43	84
13	3	178/180 (99%)	173 (97%)	5 (3%)	56	89
13	M	178/180 (99%)	175 (98%)	3 (2%)	73	94
13	a	178/180 (99%)	175 (98%)	3 (2%)	73	94
13	o	178/180 (99%)	174 (98%)	4 (2%)	64	91
14	4	159/162 (98%)	159 (100%)	0	100	100
14	N	159/162 (98%)	157 (99%)	2 (1%)	80	95
14	b	159/162 (98%)	158 (99%)	1 (1%)	92	98
14	p	159/162 (98%)	156 (98%)	3 (2%)	69	93
All	All	10392/10772 (96%)	10097 (97%)	295 (3%)	56	89

5 of 295 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Y	176	LEU
5	g	38	LEU
9	y	144	GLN
13	a	46	ASN
2	d	44	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.