



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:57 PM GMT

PDB ID : 3UNB  
Title : Mouse constitutive 20S proteasome in complex with PR-957  
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.  
Deposited on : 2011-11-15  
Resolution : 2.90 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

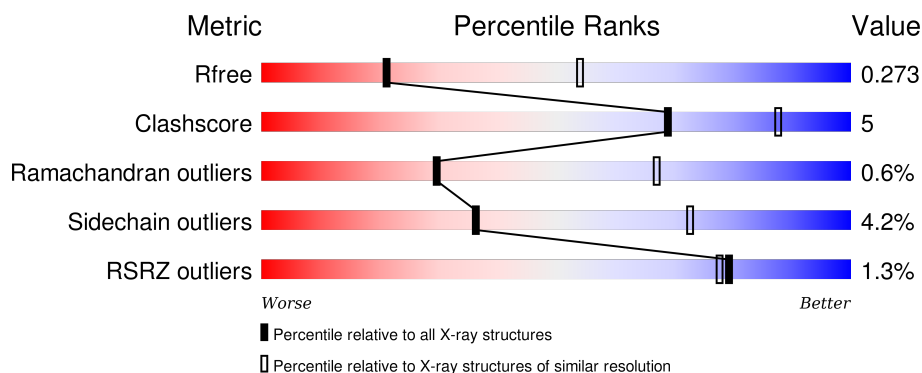
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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>83%</div> <div>15%</div> <div>.</div> </div>
1	O	234	<div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	c	234	<div> <div>95%</div> <div>.</div> <div>.</div> </div>
1	q	234	<div> <div>94%</div> <div>.</div> <div>.</div> </div>
2	B	261	<div> <div>82%</div> <div>12%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
8	j	234	 4% 89% 5% 6%
8	x	234	 89% 5% 6%
9	I	205	 87% 12%
9	W	205	 87% 12%
9	k	205	 95%
9	y	205	 2% 96%
10	J	201	 88% 9%
10	X	201	 85% 11%
10	l	201	 95%
10	z	201	 94%
11	1	205	 82% 14%
11	K	205	 85% 12%
11	Y	205	 83% 14%
11	m	205	 95%
12	2	213	 87% 12%
12	L	213	 91% 9%
12	Z	213	 89% 11%
12	n	213	 98%
13	3	219	 82% 16%
13	M	219	 88% 10%
13	a	219	 95%
13	o	219	 95%
14	4	205	 93% 6%
14	N	205	 2% 89% 9%
14	b	205	 95%

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Mol	Chain	Length	Quality of chain
14	p	205	<div><div></div><div>2%</div><div>96%</div><div></div><div>..</div></div>

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 99236 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	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	O	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	c	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	q	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	GLU	CONFLICT	UNP P49722
O	2	LYS	GLU	CONFLICT	UNP P49722
c	2	LYS	GLU	CONFLICT	UNP P49722
q	2	LYS	GLU	CONFLICT	UNP P49722

- 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 1881	C 1182	N 332	O 362	S 5	0	0	0
3	Q	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0
3	e	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0
3	s	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	45	ALA	GLU	CONFLICT	UNP Q9Z2U0
Q	45	ALA	GLU	CONFLICT	UNP Q9Z2U0
e	45	ALA	GLU	CONFLICT	UNP Q9Z2U0
s	45	ALA	GLU	CONFLICT	UNP Q9Z2U0

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

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

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

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

- 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	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	U	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	i	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	w	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

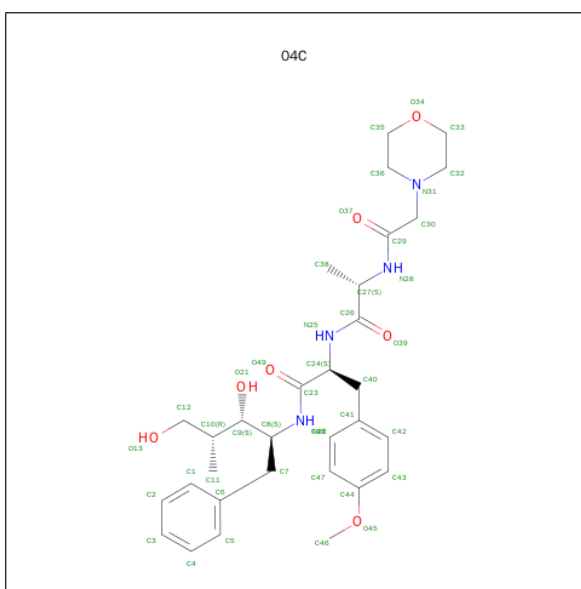
- Molecule 13 is a protein called Proteasome subunit beta type-4.

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			
14	4	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			

- Molecule 15 is 1,2,4-TRIDEOXY-4-METHYL-2-{[N-(MORPHOLIN-4-YLACETYL)-L-ALANYL-O-METHYL-L-TYROSYL]AMINO}-1-PHENYL-D-XYLITOL (three-letter code: 04C) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>4</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			42	31	4	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			42	31	4	7		
15	N	1	Total	C	N	O	0	0
			42	31	4	7		
15	V	1	Total	C	N	O	0	0
			42	31	4	7		
15	Y	1	Total	C	N	O	0	0
			42	31	4	7		
15	b	1	Total	C	N	O	0	0
			42	31	4	7		
15	j	1	Total	C	N	O	0	0
			42	31	4	7		
15	m	1	Total	C	N	O	0	0
			42	31	4	7		
15	p	1	Total	C	N	O	0	0
			42	31	4	7		
15	x	1	Total	C	N	O	0	0
			42	31	4	7		
15	1	1	Total	C	N	O	0	0
			42	31	4	7		
15	4	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	19	Total	O	0	0
			19	19		
16	B	24	Total	O	0	0
			24	24		
16	C	13	Total	O	0	0
			13	13		
16	D	16	Total	O	0	0
			16	16		
16	E	21	Total	O	0	0
			21	21		
16	F	20	Total	O	0	0
			20	20		
16	G	22	Total	O	0	0
			22	22		
16	H	31	Total	O	0	0
			31	31		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	32	Total 32	O 32	0	0
16	J	25	Total 25	O 25	0	0
16	K	28	Total 28	O 28	0	0
16	L	23	Total 23	O 23	0	0
16	M	27	Total 27	O 27	0	0
16	N	33	Total 33	O 33	0	0
16	O	33	Total 33	O 33	0	0
16	P	38	Total 38	O 38	0	0
16	Q	16	Total 16	O 16	0	0
16	R	19	Total 19	O 19	0	0
16	S	25	Total 25	O 25	0	0
16	T	25	Total 25	O 25	0	0
16	U	37	Total 37	O 37	0	0
16	V	35	Total 35	O 35	0	0
16	W	37	Total 37	O 37	0	0
16	X	33	Total 33	O 33	0	0
16	Y	16	Total 16	O 16	0	0
16	Z	32	Total 32	O 32	0	0
16	a	33	Total 33	O 33	0	0
16	b	40	Total 40	O 40	0	0
16	c	21	Total 21	O 21	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	d	19	Total 19	O 19	0	0
16	e	14	Total 14	O 14	0	0
16	f	13	Total 13	O 13	0	0
16	g	15	Total 15	O 15	0	0
16	h	19	Total 19	O 19	0	0
16	i	29	Total 29	O 29	0	0
16	j	25	Total 25	O 25	0	0
16	k	30	Total 30	O 30	0	0
16	l	22	Total 22	O 22	0	0
16	m	20	Total 20	O 20	0	0
16	n	29	Total 29	O 29	0	0
16	o	27	Total 27	O 27	0	0
16	p	32	Total 32	O 32	0	0
16	q	26	Total 26	O 26	0	0
16	r	34	Total 34	O 34	0	0
16	s	19	Total 19	O 19	0	0
16	t	17	Total 17	O 17	0	0
16	u	27	Total 27	O 27	0	0
16	v	31	Total 31	O 31	0	0
16	w	27	Total 27	O 27	0	0
16	x	34	Total 34	O 34	0	0

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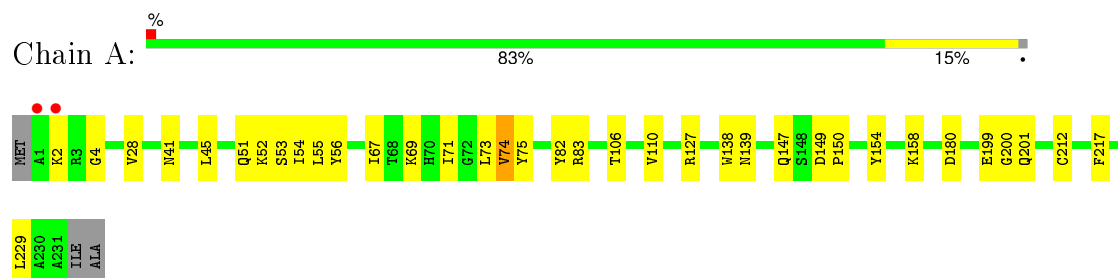
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	y	32	Total 32	O 32	0	0
16	z	38	Total 38	O 38	0	0
16	1	27	Total 27	O 27	0	0
16	2	33	Total 33	O 33	0	0
16	3	37	Total 37	O 37	0	0
16	4	30	Total 30	O 30	0	0

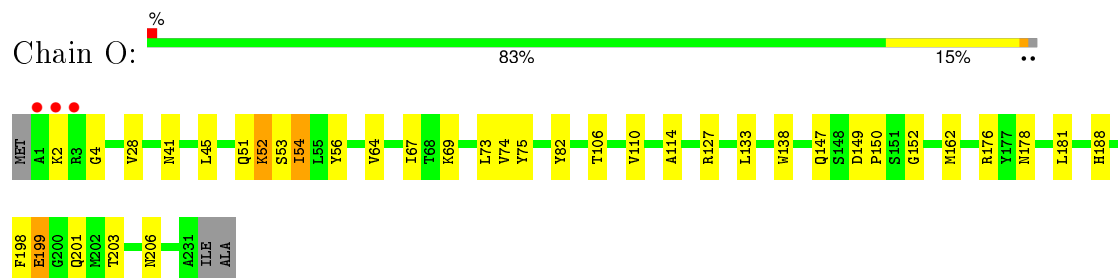
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

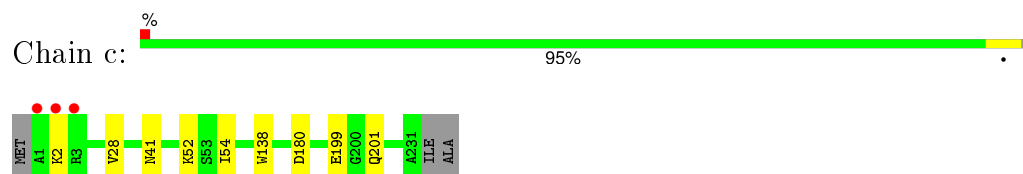
- Molecule 1: Proteasome subunit alpha type-2



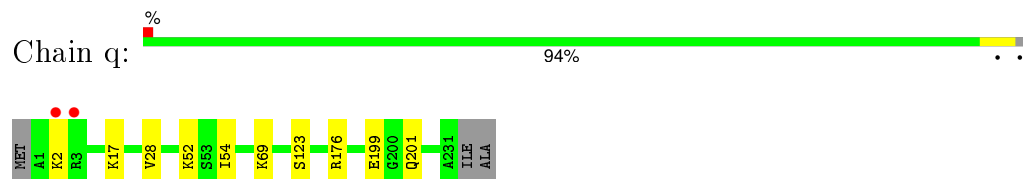
- Molecule 1: Proteasome subunit alpha type-2



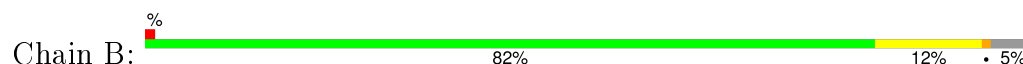
- Molecule 1: Proteasome subunit alpha type-2

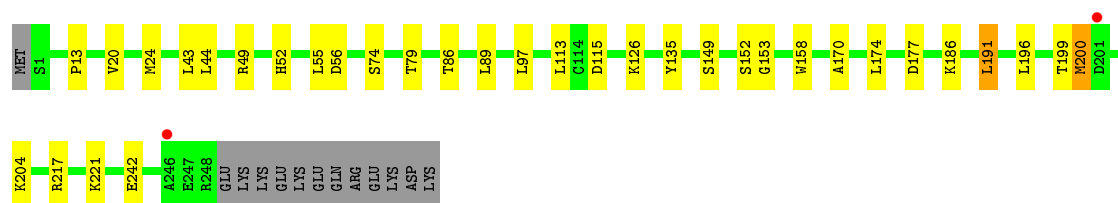


- Molecule 1: Proteasome subunit alpha type-2

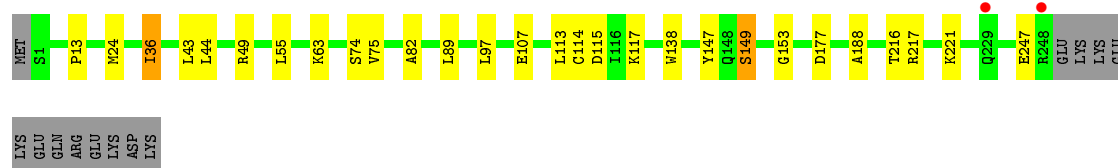
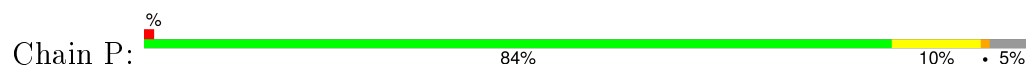


- Molecule 2: Proteasome subunit alpha type-4





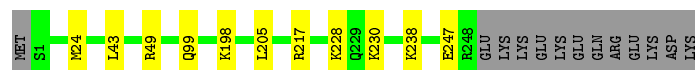
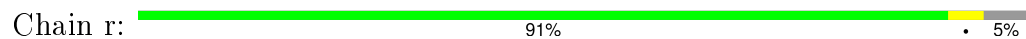
• Molecule 2: Proteasome subunit alpha type-4



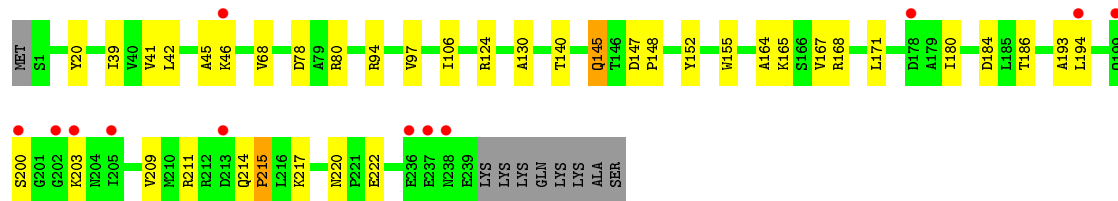
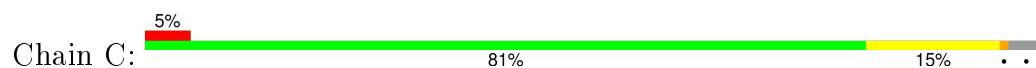
• Molecule 2: Proteasome subunit alpha type-4



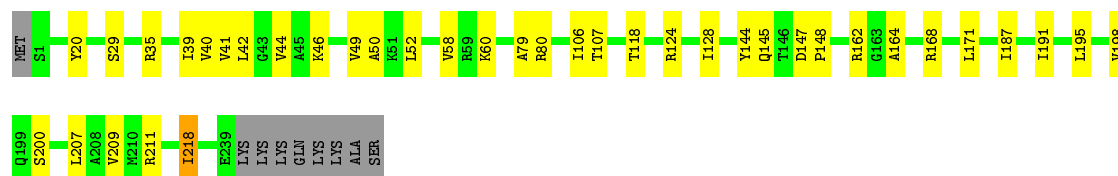
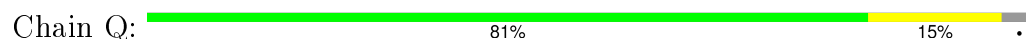
• Molecule 2: Proteasome subunit alpha type-4



• Molecule 3: Proteasome subunit alpha type-7

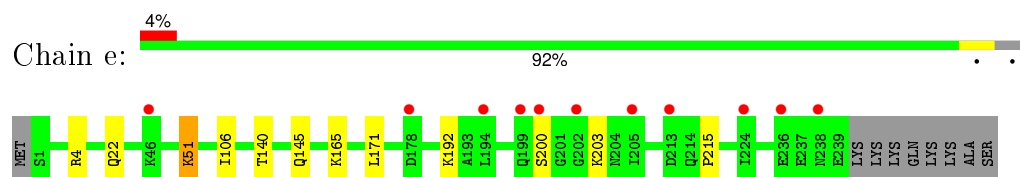


• Molecule 3: Proteasome subunit alpha type-7

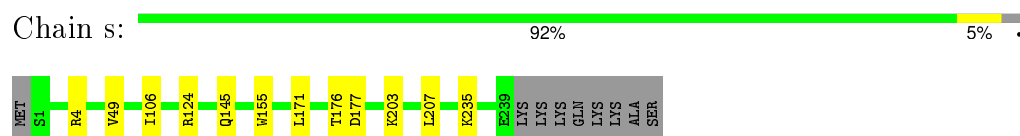




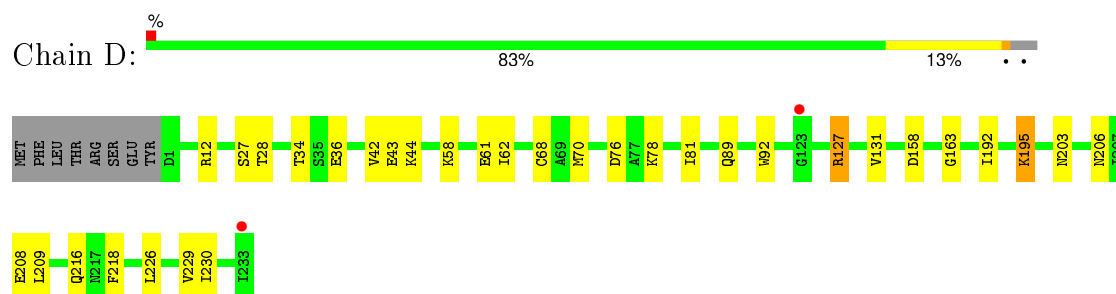
- Molecule 3: Proteasome subunit alpha type-7



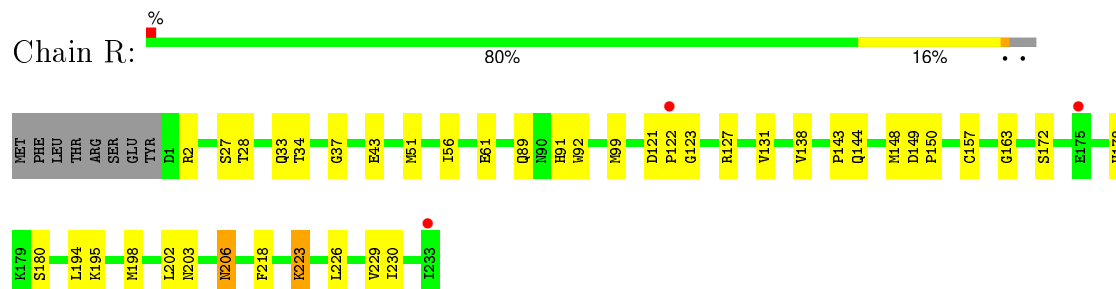
- Molecule 3: Proteasome subunit alpha type-7



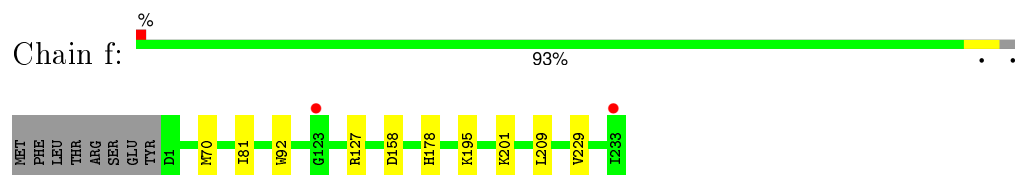
- Molecule 4: Proteasome subunit alpha type-5



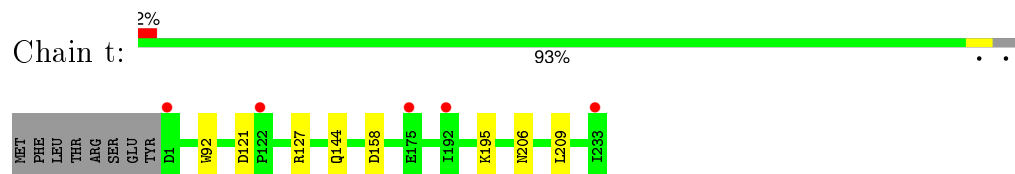
- Molecule 4: Proteasome subunit alpha type-5



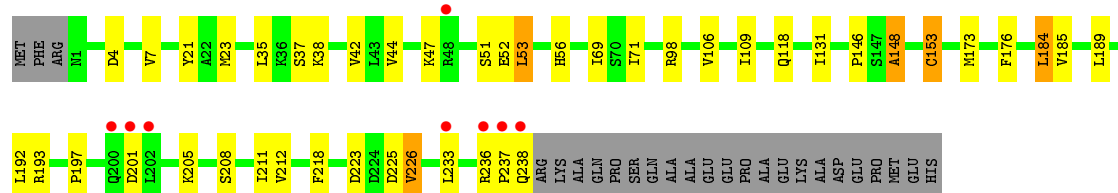
- Molecule 4: Proteasome subunit alpha type-5



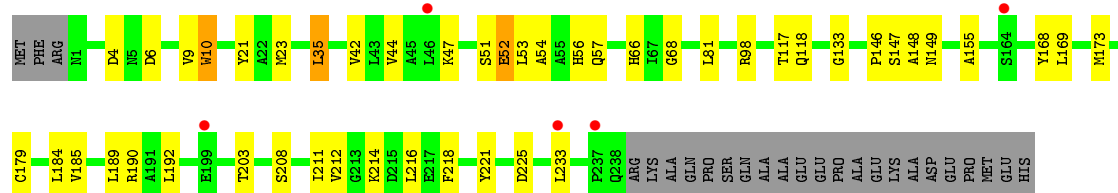
- Molecule 4: Proteasome subunit alpha type-5



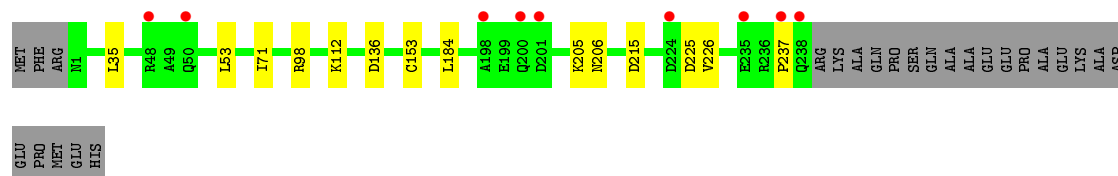
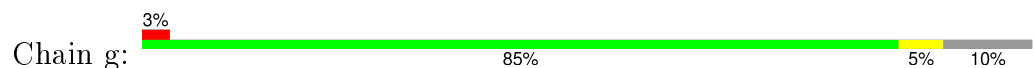
- Molecule 5: Proteasome subunit alpha type-1



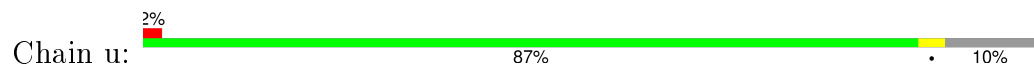
- Molecule 5: Proteasome subunit alpha type-1



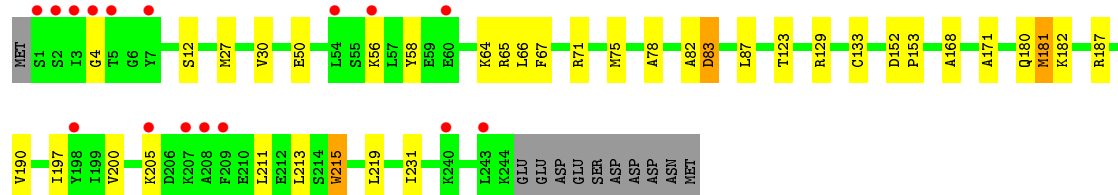
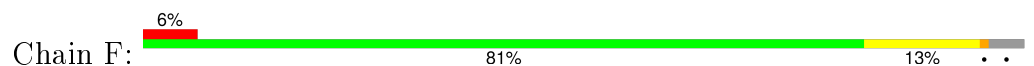
- Molecule 5: Proteasome subunit alpha type-1



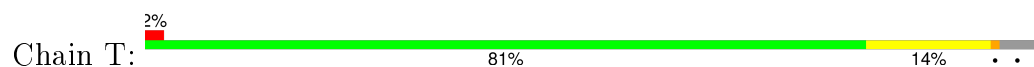
- Molecule 5: Proteasome subunit alpha type-1

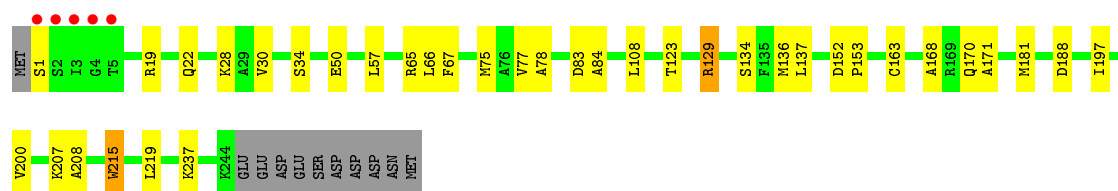


- Molecule 6: Proteasome subunit alpha type-3

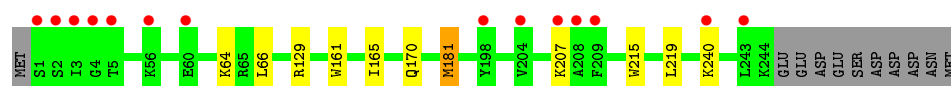


- Molecule 6: Proteasome subunit alpha type-3

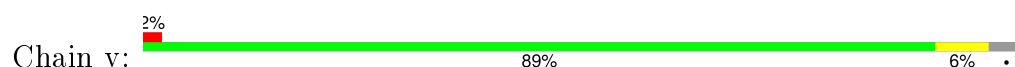




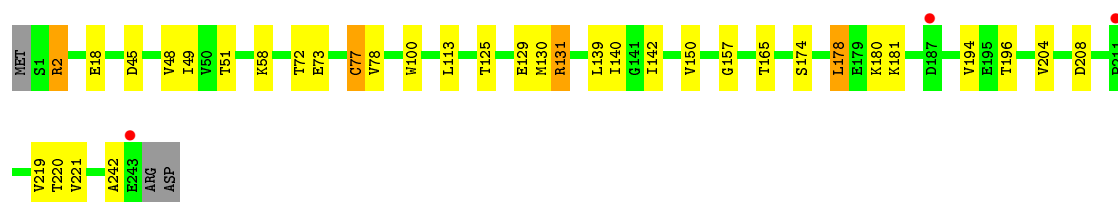
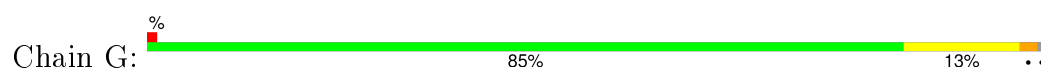
- Molecule 6: Proteasome subunit alpha type-3



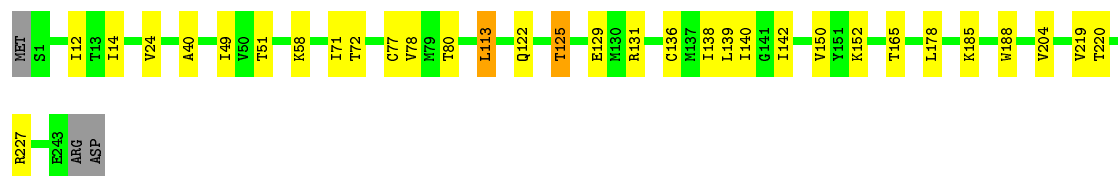
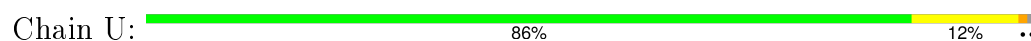
- Molecule 6: Proteasome subunit alpha type-3



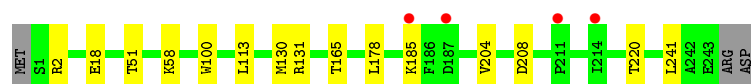
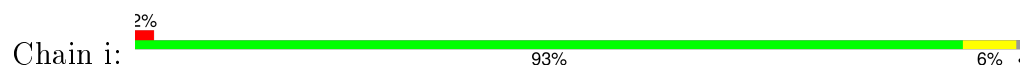
- Molecule 7: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-6




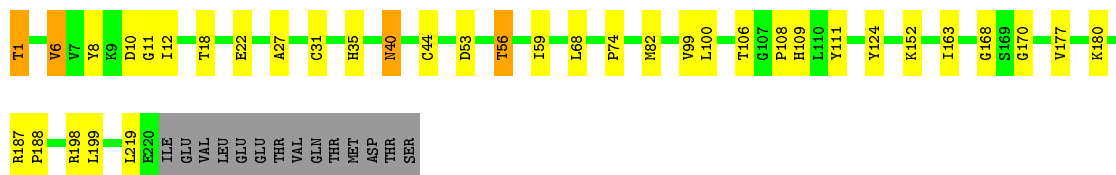
- Molecule 7: Proteasome subunit alpha type-6

Chain w:  94% . .




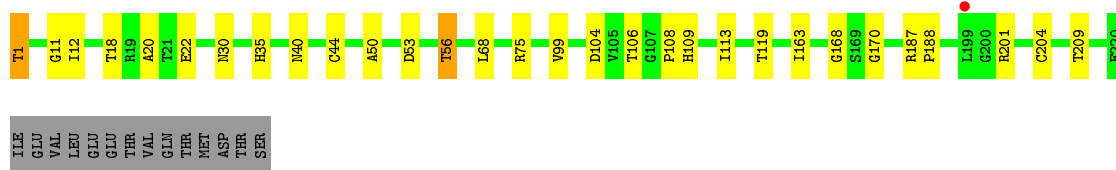
- Molecule 8: Proteasome subunit beta type-7

Chain H:  78% 14% 6%




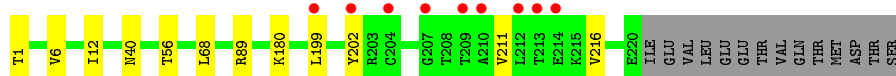
- Molecule 8: Proteasome subunit beta type-7

Chain V:  81% 12% 6%




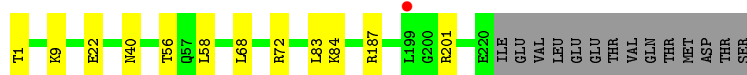
- Molecule 8: Proteasome subunit beta type-7

Chain j:  4% 89% 5% 6%




- Molecule 8: Proteasome subunit beta type-7

Chain x:  89% 5% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  87% 12%



- Molecule 9: Proteasome subunit beta type-3

Chain W:  87% 12%



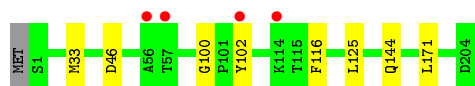
- Molecule 9: Proteasome subunit beta type-3

Chain k: 95%



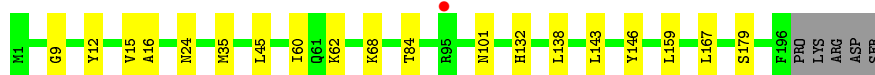
- Molecule 9: Proteasome subunit beta type-3

Chain y: 96%



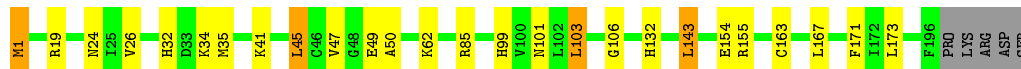
- Molecule 10: Proteasome subunit beta type-2

Chain J: 88% 9%



- Molecule 10: Proteasome subunit beta type-2

Chain X: 85% 11%



- Molecule 10: Proteasome subunit beta type-2

Chain l: 95%



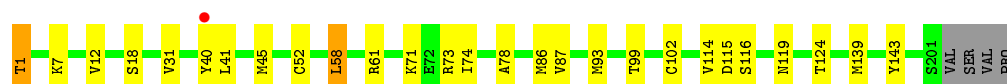
- Molecule 10: Proteasome subunit beta type-2

Chain z: 94%

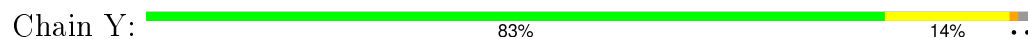


- Molecule 11: Proteasome subunit beta type-5

Chain K: 85% 12%



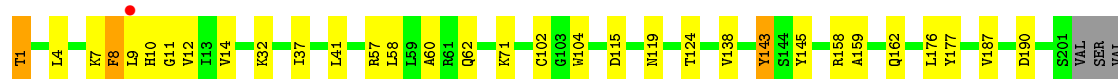
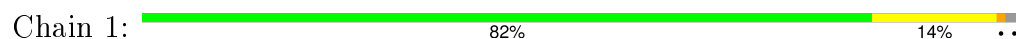
• Molecule 11: Proteasome subunit beta type-5



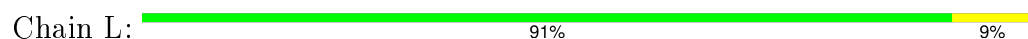
• Molecule 11: Proteasome subunit beta type-5



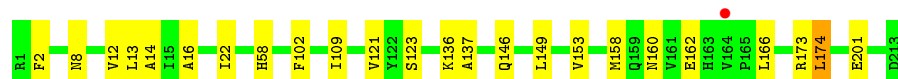
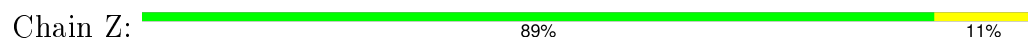
• Molecule 11: Proteasome subunit beta type-5



• Molecule 12: Proteasome subunit beta type-1



• Molecule 12: Proteasome subunit beta type-1



• Molecule 12: Proteasome subunit beta type-1





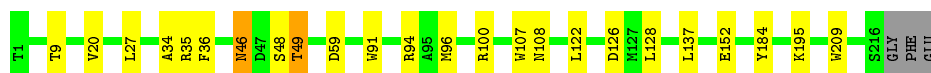
- Molecule 12: Proteasome subunit beta type-1

Chain 2: 87% 12%



- Molecule 13: Proteasome subunit beta type-4

Chain M: 88% 10%



- Molecule 13: Proteasome subunit beta type-4

Chain a: 95%



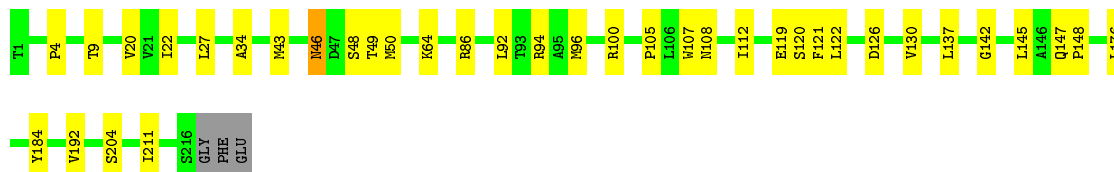
- Molecule 13: Proteasome subunit beta type-4

Chain o: 95%



- Molecule 13: Proteasome subunit beta type-4

Chain 3: 82% 16%



- Molecule 14: Proteasome subunit beta type-6

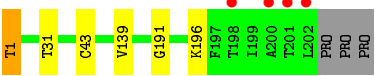
Chain N: 89% 9% 2%



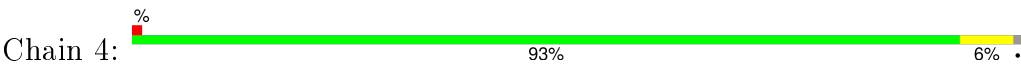
- Molecule 14: Proteasome subunit beta type-6



● 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, $\alpha$ , $\beta$ , $\gamma$	171.72Å 198.59Å 226.75Å 90.00° 106.59° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 49.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-2.90) 96.0 (49.19-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, $R_{free}$	0.230 , 0.273 0.230 , 0.273	Depositor DCC
$R_{free}$ test set	15336 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	4 of 308934 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	99236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.11 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.3244e-11. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 04C

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	0.39	1/1845 (0.1%)	0.49	0/2498
1	O	0.39	1/1845 (0.1%)	0.48	0/2498
1	c	0.39	1/1845 (0.1%)	0.48	0/2498
1	q	0.39	0/1845	0.47	0/2498
2	B	0.37	1/1980 (0.1%)	0.48	0/2667
2	P	0.37	1/1980 (0.1%)	0.48	0/2667
2	d	0.37	0/1980	0.48	0/2667
2	r	0.37	0/1980	0.48	0/2667
3	C	0.33	0/1908	0.47	0/2576
3	Q	0.34	0/1908	0.48	0/2576
3	e	0.33	0/1908	0.47	0/2576
3	s	0.34	1/1908 (0.1%)	0.47	0/2576
4	D	0.36	1/1805 (0.1%)	0.47	0/2437
4	R	0.36	1/1805 (0.1%)	0.46	0/2437
4	f	0.36	1/1805 (0.1%)	0.47	0/2437
4	t	0.37	0/1805	0.47	0/2437
5	E	0.37	0/1907	0.49	0/2578
5	S	0.38	1/1907 (0.1%)	0.51	0/2578
5	g	0.37	0/1907	0.48	0/2578
5	u	0.38	1/1907 (0.1%)	0.50	0/2578
6	F	0.39	1/1938 (0.1%)	0.48	0/2608
6	T	0.38	1/1938 (0.1%)	0.48	0/2608
6	h	0.38	1/1938 (0.1%)	0.48	0/2608
6	v	0.39	2/1938 (0.1%)	0.48	0/2608
7	G	0.37	1/1924 (0.1%)	0.48	0/2600
7	U	0.38	1/1924 (0.1%)	0.49	0/2600
7	i	0.37	1/1924 (0.1%)	0.48	0/2600
7	w	0.38	1/1924 (0.1%)	0.48	0/2600
8	H	0.35	0/1683	0.51	1/2276 (0.0%)
8	V	0.37	1/1683 (0.1%)	0.51	0/2276
8	j	0.33	0/1683	0.52	0/2276
8	x	0.36	1/1683 (0.1%)	0.52	1/2276 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	I	0.34	0/1621	0.49	0/2185
9	W	0.35	0/1621	0.49	0/2185
9	k	0.34	0/1621	0.48	0/2185
9	y	0.35	0/1621	0.50	0/2185
10	J	0.33	0/1602	0.49	0/2167
10	X	0.33	0/1602	0.49	0/2167
10	l	0.33	0/1602	0.49	0/2167
10	z	0.33	0/1602	0.49	0/2167
11	1	0.44	1/1588 (0.1%)	0.50	0/2145
11	K	0.44	1/1588 (0.1%)	0.50	0/2145
11	Y	0.46	2/1588 (0.1%)	0.48	0/2145
11	m	0.45	1/1588 (0.1%)	0.50	0/2145
12	2	0.32	0/1685	0.48	0/2271
12	L	0.33	0/1685	0.48	0/2271
12	Z	0.33	0/1685	0.48	0/2271
12	n	0.33	0/1685	0.47	0/2271
13	3	0.40	0/1718	0.50	0/2325
13	M	0.41	3/1718 (0.2%)	0.50	0/2325
13	a	0.41	1/1718 (0.1%)	0.51	0/2325
13	o	0.40	1/1718 (0.1%)	0.48	0/2325
14	4	0.39	1/1546 (0.1%)	0.48	0/2094
14	N	0.39	2/1546 (0.1%)	0.48	0/2094
14	b	0.39	1/1546 (0.1%)	0.49	0/2094
14	p	0.39	1/1546 (0.1%)	0.48	0/2094
All	All	0.37	37/99000 (0.0%)	0.49	2/133708 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
8	V	0	1
8	j	0	1
11	1	0	1
11	K	0	1
11	Y	0	1
11	m	0	1
14	4	0	1
14	N	0	1
14	b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	p	0	1
All	All	0	11

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1	THR	C-N	7.39	1.51	1.34
11	m	1	THR	C-N	7.02	1.50	1.34
11	K	1	THR	C-N	6.13	1.48	1.34
8	V	1	THR	C-N	6.04	1.48	1.34
8	x	1	THR	C-N	6.00	1.47	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	THR	C-N-CA	6.26	137.36	121.70
8	x	1	THR	C-N-CA	5.11	134.48	121.70

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	1	THR	Peptide
11	K	1	THR	Peptide
14	N	1	THR	Peptide
8	V	1	THR	Mainchain
11	Y	1	THR	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1805	21	0
1	O	1806	0	1805	21	0
1	c	1806	0	1805	0	0
1	q	1806	0	1805	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1950	0	1973	13	0
2	P	1950	0	1973	13	0
2	d	1950	0	1973	0	0
2	r	1950	0	1973	0	0
3	C	1881	0	1907	19	0
3	Q	1881	0	1907	20	0
3	e	1881	0	1907	0	0
3	s	1881	0	1907	0	0
4	D	1778	0	1767	14	0
4	R	1778	0	1767	19	0
4	f	1778	0	1767	0	0
4	t	1778	0	1767	0	0
5	E	1872	0	1859	22	0
5	S	1872	0	1859	25	0
5	g	1872	0	1859	0	0
5	u	1872	0	1859	0	0
6	F	1903	0	1894	20	0
6	T	1903	0	1894	21	0
6	h	1903	0	1894	0	0
6	v	1903	0	1894	0	0
7	G	1890	0	1900	17	0
7	U	1890	0	1900	16	0
7	i	1890	0	1900	0	0
7	w	1890	0	1900	0	0
8	H	1656	0	1682	23	0
8	V	1656	0	1683	15	0
8	j	1656	0	1682	0	0
8	x	1656	0	1683	0	0
9	I	1592	0	1612	13	0
9	W	1592	0	1612	15	0
9	k	1592	0	1612	0	0
9	y	1592	0	1612	0	0
10	J	1570	0	1573	12	0
10	X	1570	0	1573	13	0
10	l	1570	0	1573	0	0
10	z	1570	0	1573	0	0
11	1	1557	0	1523	14	0
11	K	1557	0	1524	14	0
11	Y	1557	0	1523	12	0
11	m	1557	0	1524	0	0
12	2	1654	0	1652	16	0
12	L	1654	0	1652	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1654	0	1652	12	0
12	n	1654	0	1652	0	0
13	3	1685	0	1664	23	0
13	M	1685	0	1664	11	0
13	a	1685	0	1664	0	0
13	o	1685	0	1664	0	0
14	4	1519	0	1485	5	0
14	N	1519	0	1486	9	0
14	b	1519	0	1486	0	0
14	p	1519	0	1485	0	0
15	1	42	0	42	0	0
15	4	42	0	42	2	0
15	H	42	0	42	5	0
15	K	42	0	42	0	0
15	N	42	0	42	1	0
15	V	42	0	42	3	0
15	Y	42	0	42	0	0
15	b	42	0	42	0	0
15	j	42	0	42	0	0
15	m	42	0	42	0	0
15	p	42	0	42	0	0
15	x	42	0	42	0	0
16	1	27	0	0	1	0
16	2	33	0	0	0	0
16	3	37	0	0	2	0
16	4	30	0	0	0	0
16	A	19	0	0	1	0
16	B	24	0	0	0	0
16	C	13	0	0	0	0
16	D	16	0	0	0	0
16	E	21	0	0	1	0
16	F	20	0	0	0	0
16	G	22	0	0	0	0
16	H	31	0	0	0	0
16	I	32	0	0	0	0
16	J	25	0	0	0	0
16	K	28	0	0	1	0
16	L	23	0	0	0	0
16	M	27	0	0	0	0
16	N	33	0	0	0	0
16	O	33	0	0	1	0
16	P	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	16	0	0	0	0
16	R	19	0	0	0	0
16	S	25	0	0	0	0
16	T	25	0	0	0	0
16	U	37	0	0	0	0
16	V	35	0	0	0	0
16	W	37	0	0	0	0
16	X	33	0	0	2	0
16	Y	16	0	0	0	0
16	Z	32	0	0	0	0
16	a	33	0	0	0	0
16	b	40	0	0	0	0
16	c	21	0	0	0	0
16	d	19	0	0	0	0
16	e	14	0	0	0	0
16	f	13	0	0	0	0
16	g	15	0	0	0	0
16	h	19	0	0	0	0
16	i	29	0	0	0	0
16	j	25	0	0	0	0
16	k	30	0	0	0	0
16	l	22	0	0	0	0
16	m	20	0	0	0	0
16	n	29	0	0	0	0
16	o	27	0	0	0	0
16	p	32	0	0	0	0
16	q	26	0	0	0	0
16	r	34	0	0	0	0
16	s	19	0	0	0	0
16	t	17	0	0	0	0
16	u	27	0	0	0	0
16	v	31	0	0	0	0
16	w	27	0	0	0	0
16	x	34	0	0	0	0
16	y	32	0	0	0	0
16	z	38	0	0	0	0
All	All	99236	0	97694	443	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 5.

The worst 5 of 443 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)
10:J:60:ILE:HG21	10:J:84:THR:HG22	1.36	1.07
8:V:187:ARG:HB3	8:V:188:PRO:HD3	1.56	0.86
8:H:187:ARG:HB3	8:H:188:PRO:HD3	1.60	0.83
12:L:8:ASN:HD22	12:L:58:HIS:H	1.28	0.82
1:A:4:GLY:HA2	7:G:129:GLU:HG2	1.61	0.82

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	229/234 (98%)	214 (93%)	9 (4%)	6 (3%)	7	26
1	O	229/234 (98%)	215 (94%)	9 (4%)	5 (2%)	8	31
1	c	229/234 (98%)	217 (95%)	7 (3%)	5 (2%)	8	31
1	q	229/234 (98%)	216 (94%)	9 (4%)	4 (2%)	11	38
2	B	246/261 (94%)	239 (97%)	7 (3%)	0	100	100
2	P	246/261 (94%)	238 (97%)	8 (3%)	0	100	100
2	d	246/261 (94%)	237 (96%)	9 (4%)	0	100	100
2	r	246/261 (94%)	239 (97%)	6 (2%)	1 (0%)	39	74
3	C	237/248 (96%)	220 (93%)	15 (6%)	2 (1%)	24	60
3	Q	237/248 (96%)	227 (96%)	8 (3%)	2 (1%)	24	60
3	e	237/248 (96%)	224 (94%)	10 (4%)	3 (1%)	15	46
3	s	237/248 (96%)	225 (95%)	11 (5%)	1 (0%)	39	74
4	D	231/241 (96%)	222 (96%)	9 (4%)	0	100	100
4	R	231/241 (96%)	220 (95%)	10 (4%)	1 (0%)	39	74
4	f	231/241 (96%)	217 (94%)	14 (6%)	0	100	100
4	t	231/241 (96%)	219 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	236/263 (90%)	223 (94%)	10 (4%)	3 (1%)	15	46
5	S	236/263 (90%)	219 (93%)	15 (6%)	2 (1%)	24	60
5	g	236/263 (90%)	220 (93%)	15 (6%)	1 (0%)	39	74
5	u	236/263 (90%)	221 (94%)	14 (6%)	1 (0%)	39	74
6	F	242/255 (95%)	232 (96%)	8 (3%)	2 (1%)	24	60
6	T	242/255 (95%)	234 (97%)	8 (3%)	0	100	100
6	h	242/255 (95%)	235 (97%)	5 (2%)	2 (1%)	24	60
6	v	242/255 (95%)	233 (96%)	7 (3%)	2 (1%)	24	60
7	G	241/246 (98%)	235 (98%)	3 (1%)	3 (1%)	16	48
7	U	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	i	241/246 (98%)	234 (97%)	5 (2%)	2 (1%)	24	60
7	w	241/246 (98%)	234 (97%)	6 (2%)	1 (0%)	39	74
8	H	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
8	V	218/234 (93%)	210 (96%)	8 (4%)	0	100	100
8	j	218/234 (93%)	212 (97%)	6 (3%)	0	100	100
8	x	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	34	71
9	I	202/205 (98%)	188 (93%)	9 (4%)	5 (2%)	7	27
9	W	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	34	71
9	k	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	13	42
9	y	202/205 (98%)	183 (91%)	16 (8%)	3 (2%)	13	42
10	J	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	34	71
10	X	194/201 (96%)	188 (97%)	4 (2%)	2 (1%)	19	54
10	l	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	34	71
10	z	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	34	71
11	1	199/205 (97%)	192 (96%)	7 (4%)	0	100	100
11	K	199/205 (97%)	193 (97%)	6 (3%)	0	100	100
11	Y	199/205 (97%)	196 (98%)	3 (2%)	0	100	100
11	m	199/205 (97%)	192 (96%)	7 (4%)	0	100	100
12	2	211/213 (99%)	204 (97%)	5 (2%)	2 (1%)	21	57
12	L	211/213 (99%)	204 (97%)	6 (3%)	1 (0%)	34	71
12	Z	211/213 (99%)	200 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	n	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
13	3	214/219 (98%)	200 (94%)	13 (6%)	1 (0%)	34	71
13	M	214/219 (98%)	203 (95%)	10 (5%)	1 (0%)	34	71
13	a	214/219 (98%)	202 (94%)	11 (5%)	1 (0%)	34	71
13	o	214/219 (98%)	206 (96%)	7 (3%)	1 (0%)	34	71
14	4	200/205 (98%)	193 (96%)	7 (4%)	0	100	100
14	N	200/205 (98%)	191 (96%)	8 (4%)	1 (0%)	34	71
14	b	200/205 (98%)	189 (94%)	10 (5%)	1 (0%)	34	71
14	p	200/205 (98%)	188 (94%)	11 (6%)	1 (0%)	34	71
All	All	12400/12920 (96%)	11841 (96%)	482 (4%)	77 (1%)	30	67

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	181	MET
14	N	191	GLY
1	O	54	ILE
5	S	52	GLU
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%)	184 (97%)	5 (3%)	54	85
1	O	189/191 (99%)	185 (98%)	4 (2%)	61	88
1	c	189/191 (99%)	186 (98%)	3 (2%)	70	91
1	q	189/191 (99%)	183 (97%)	6 (3%)	46	81
2	B	208/221 (94%)	194 (93%)	14 (7%)	20	50
2	P	208/221 (94%)	195 (94%)	13 (6%)	22	54
2	d	208/221 (94%)	196 (94%)	12 (6%)	25	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	r	208/221 (94%)	198 (95%)	10 (5%)	31	67
3	C	202/210 (96%)	191 (95%)	11 (5%)	27	62
3	Q	202/210 (96%)	195 (96%)	7 (4%)	43	78
3	e	202/210 (96%)	192 (95%)	10 (5%)	30	65
3	s	202/210 (96%)	192 (95%)	10 (5%)	30	65
4	D	195/203 (96%)	185 (95%)	10 (5%)	29	65
4	R	195/203 (96%)	185 (95%)	10 (5%)	29	65
4	f	195/203 (96%)	186 (95%)	9 (5%)	33	69
4	t	195/203 (96%)	187 (96%)	8 (4%)	37	73
5	E	204/224 (91%)	192 (94%)	12 (6%)	24	58
5	S	204/224 (91%)	195 (96%)	9 (4%)	35	70
5	g	204/224 (91%)	191 (94%)	13 (6%)	22	53
5	u	204/224 (91%)	197 (97%)	7 (3%)	44	79
6	F	200/211 (95%)	192 (96%)	8 (4%)	38	74
6	T	200/211 (95%)	190 (95%)	10 (5%)	30	65
6	h	200/211 (95%)	191 (96%)	9 (4%)	34	70
6	v	200/211 (95%)	187 (94%)	13 (6%)	21	52
7	G	207/210 (99%)	196 (95%)	11 (5%)	28	63
7	U	207/210 (99%)	195 (94%)	12 (6%)	25	58
7	i	207/210 (99%)	195 (94%)	12 (6%)	25	58
7	w	207/210 (99%)	198 (96%)	9 (4%)	35	71
8	H	181/195 (93%)	174 (96%)	7 (4%)	39	75
8	V	181/195 (93%)	174 (96%)	7 (4%)	39	75
8	j	181/195 (93%)	170 (94%)	11 (6%)	23	56
8	x	181/195 (93%)	171 (94%)	10 (6%)	27	61
9	I	174/175 (99%)	171 (98%)	3 (2%)	68	91
9	W	174/175 (99%)	170 (98%)	4 (2%)	58	87
9	k	174/175 (99%)	168 (97%)	6 (3%)	44	79
9	y	174/175 (99%)	169 (97%)	5 (3%)	50	83
10	J	166/171 (97%)	164 (99%)	2 (1%)	78	94
10	X	166/171 (97%)	157 (95%)	9 (5%)	27	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	l	166/171 (97%)	161 (97%)	5 (3%)	48	83
10	z	166/171 (97%)	159 (96%)	7 (4%)	36	73
11	1	157/161 (98%)	147 (94%)	10 (6%)	22	53
11	K	157/161 (98%)	152 (97%)	5 (3%)	46	81
11	Y	157/161 (98%)	147 (94%)	10 (6%)	22	53
11	m	157/161 (98%)	151 (96%)	6 (4%)	40	76
12	2	178/178 (100%)	173 (97%)	5 (3%)	51	84
12	L	178/178 (100%)	170 (96%)	8 (4%)	34	70
12	Z	178/178 (100%)	171 (96%)	7 (4%)	39	75
12	n	178/178 (100%)	173 (97%)	5 (3%)	51	84
13	3	178/180 (99%)	173 (97%)	5 (3%)	51	84
13	M	178/180 (99%)	172 (97%)	6 (3%)	44	79
13	a	178/180 (99%)	172 (97%)	6 (3%)	44	79
13	o	178/180 (99%)	172 (97%)	6 (3%)	44	79
14	4	159/162 (98%)	156 (98%)	3 (2%)	65	89
14	N	159/162 (98%)	156 (98%)	3 (2%)	65	89
14	b	159/162 (98%)	153 (96%)	6 (4%)	40	76
14	p	159/162 (98%)	155 (98%)	4 (2%)	55	85
All	All	10392/10768 (96%)	9954 (96%)	438 (4%)	36	73

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Y	186	ARG
4	f	81	ILE
9	y	102	TYR
12	Z	160	ASN
2	d	24	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 160 such sidechains are listed below:

Mol	Chain	Res	Type
13	a	46	ASN
5	g	143	GLN
10	z	71	ASN

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Mol	Chain	Res	Type
13	a	157	GLN
3	e	91	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
15	04C	1	301	11	43,44,44	1.80	7 (16%)	55,58,58	0.99	4 (7%)
15	04C	4	301	14	43,44,44	1.21	2 (4%)	55,58,58	1.01	3 (5%)
15	04C	H	301	8	43,44,44	1.30	5 (11%)	55,58,58	0.88	3 (5%)
15	04C	K	301	11	43,44,44	1.22	3 (6%)	55,58,58	1.22	2 (3%)
15	04C	N	301	14	43,44,44	1.20	3 (6%)	55,58,58	1.10	3 (5%)
15	04C	V	301	8	43,44,44	1.24	4 (9%)	55,58,58	0.90	3 (5%)
15	04C	Y	301	11	43,44,44	1.33	4 (9%)	55,58,58	1.10	3 (5%)
15	04C	b	301	14	43,44,44	1.16	2 (4%)	55,58,58	1.02	3 (5%)
15	04C	j	301	8	43,44,44	1.26	4 (9%)	55,58,58	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	04C	m	301	11	43,44,44	1.22	3 (6%)	55,58,58	1.11	2 (3%)
15	04C	p	301	14	43,44,44	1.24	3 (6%)	55,58,58	1.13	4 (7%)
15	04C	x	301	8	43,44,44	1.21	3 (6%)	55,58,58	0.93	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	04C	l	301	11	-	0/44/52/52	0/3/3/3
15	04C	4	301	14	-	0/44/52/52	0/3/3/3
15	04C	H	301	8	-	0/44/52/52	0/3/3/3
15	04C	K	301	11	-	0/44/52/52	0/3/3/3
15	04C	N	301	14	-	0/44/52/52	0/3/3/3
15	04C	V	301	8	-	0/44/52/52	0/3/3/3
15	04C	Y	301	11	-	0/44/52/52	0/3/3/3
15	04C	b	301	14	-	0/44/52/52	0/3/3/3
15	04C	j	301	8	-	0/44/52/52	0/3/3/3
15	04C	m	301	11	-	0/44/52/52	0/3/3/3
15	04C	p	301	14	-	0/44/52/52	0/3/3/3
15	04C	x	301	8	-	0/44/52/52	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	l	301	04C	O45-C44	-8.26	1.19	1.37
15	H	301	04C	O45-C44	-2.46	1.32	1.37
15	l	301	04C	C40-C41	2.15	1.56	1.51
15	l	301	04C	C5-C6	2.17	1.43	1.38
15	l	301	04C	C48-C41	2.20	1.43	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	301	04C	C11-C10-C12	-5.39	102.76	109.86
15	p	301	04C	C11-C10-C12	-4.87	103.44	109.86
15	m	301	04C	C11-C10-C12	-4.73	103.62	109.86
15	N	301	04C	C11-C10-C12	-4.72	103.63	109.86
15	b	301	04C	C11-C10-C12	-4.35	104.13	109.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	301	04C	2	0
15	H	301	04C	5	0
15	N	301	04C	1	0
15	V	301	04C	3	0

## 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	231/234 (98%)	-0.35	2 (0%) 85 84	42, 62, 99, 145	0
1	O	231/234 (98%)	-0.34	3 (1%) 79 78	40, 59, 95, 145	0
1	c	231/234 (98%)	-0.34	3 (1%) 79 78	44, 64, 99, 143	0
1	q	231/234 (98%)	-0.34	2 (0%) 85 84	39, 61, 97, 140	0
2	B	248/261 (95%)	-0.31	2 (0%) 87 86	42, 69, 115, 156	0
2	P	248/261 (95%)	-0.29	2 (0%) 87 86	34, 62, 108, 155	0
2	d	248/261 (95%)	-0.26	2 (0%) 87 86	42, 71, 112, 161	0
2	r	248/261 (95%)	-0.28	0 100 100	40, 63, 109, 143	0
3	C	239/248 (96%)	0.17	12 (5%) 32 26	47, 83, 153, 182	0
3	Q	239/248 (96%)	-0.06	0 100 100	42, 74, 129, 163	0
3	e	239/248 (96%)	0.17	11 (4%) 36 30	51, 85, 148, 175	0
3	s	239/248 (96%)	-0.05	0 100 100	45, 75, 129, 164	0
4	D	233/241 (96%)	-0.29	2 (0%) 85 84	50, 74, 104, 149	0
4	R	233/241 (96%)	-0.25	3 (1%) 79 78	43, 72, 108, 163	0
4	f	233/241 (96%)	-0.29	2 (0%) 85 84	47, 75, 108, 158	0
4	t	233/241 (96%)	-0.22	5 (2%) 67 62	47, 73, 111, 171	0
5	E	238/263 (90%)	0.01	8 (3%) 49 41	45, 81, 135, 180	0
5	S	238/263 (90%)	-0.09	5 (2%) 67 62	39, 65, 125, 160	0
5	g	238/263 (90%)	0.05	9 (3%) 44 37	48, 81, 136, 172	0
5	u	238/263 (90%)	-0.06	6 (2%) 61 55	41, 65, 126, 156	0
6	F	244/255 (95%)	-0.00	16 (6%) 22 16	44, 76, 134, 167	0
6	T	244/255 (95%)	-0.20	5 (2%) 68 64	40, 64, 106, 159	0
6	h	244/255 (95%)	0.03	14 (5%) 27 21	47, 77, 135, 156	0
6	v	244/255 (95%)	-0.20	5 (2%) 68 64	39, 65, 110, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	G	243/246 (98%)	-0.14	3 (1%) 81 78	42, 68, 108, 161	0
7	U	243/246 (98%)	-0.36	0 100 100	39, 59, 87, 121	0
7	i	243/246 (98%)	-0.12	4 (1%) 74 72	44, 70, 108, 138	0
7	w	243/246 (98%)	-0.39	0 100 100	39, 59, 88, 122	0
8	H	220/234 (94%)	-0.30	0 100 100	24, 52, 91, 127	0
8	V	220/234 (94%)	-0.36	1 (0%) 91 90	23, 49, 89, 126	0
8	j	220/234 (94%)	-0.10	9 (4%) 41 34	27, 54, 113, 146	0
8	x	220/234 (94%)	-0.29	1 (0%) 91 90	33, 54, 91, 127	0
9	I	204/205 (99%)	-0.33	1 (0%) 91 90	40, 55, 87, 119	0
9	W	204/205 (99%)	-0.35	0 100 100	35, 54, 89, 122	0
9	k	204/205 (99%)	-0.31	0 100 100	40, 56, 88, 122	0
9	y	204/205 (99%)	-0.16	4 (1%) 68 64	41, 60, 89, 126	0
10	J	196/201 (97%)	-0.36	1 (0%) 91 90	44, 59, 87, 114	0
10	X	196/201 (97%)	-0.41	0 100 100	40, 58, 85, 107	0
10	l	196/201 (97%)	-0.37	0 100 100	42, 59, 88, 112	0
10	z	196/201 (97%)	-0.37	0 100 100	40, 59, 86, 106	0
11	1	201/205 (98%)	-0.32	1 (0%) 91 90	36, 57, 88, 111	0
11	K	201/205 (98%)	-0.38	1 (0%) 91 90	38, 58, 92, 113	0
11	Y	201/205 (98%)	-0.33	1 (0%) 91 90	35, 56, 86, 109	0
11	m	201/205 (98%)	-0.34	1 (0%) 91 90	40, 59, 92, 117	0
12	2	213/213 (100%)	-0.30	1 (0%) 91 90	36, 57, 84, 135	0
12	L	213/213 (100%)	-0.24	1 (0%) 91 90	40, 56, 90, 123	0
12	Z	213/213 (100%)	-0.35	1 (0%) 91 90	37, 54, 86, 135	0
12	n	213/213 (100%)	-0.21	2 (0%) 85 84	42, 57, 91, 132	0
13	3	216/219 (98%)	-0.29	0 100 100	34, 52, 79, 101	0
13	M	216/219 (98%)	-0.37	0 100 100	36, 53, 82, 115	0
13	a	216/219 (98%)	-0.36	0 100 100	33, 49, 79, 105	0
13	o	216/219 (98%)	-0.31	0 100 100	40, 56, 84, 123	0
14	4	202/205 (98%)	-0.38	2 (0%) 84 82	31, 50, 99, 152	0
14	N	202/205 (98%)	-0.25	4 (1%) 68 64	30, 52, 91, 148	0
14	b	202/205 (98%)	-0.38	3 (1%) 76 74	30, 49, 95, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	p	202/205 (98%)	-0.24	4 (1%) 68 64	32, 53, 92, 147	0
All	All	12512/12920 (96%)	-0.24	165 (1%) 79 78	23, 62, 111, 182	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	t	233	ILE	9.3
6	T	1	SER	8.8
6	v	1	SER	8.6
8	j	212	LEU	7.3
14	N	201	THR	6.6

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	04C	Y	301	42/42	0.94	0.19	1.50	24,41,70,74	0
15	04C	l	301	42/42	0.94	0.19	1.44	24,39,71,77	0
15	04C	K	301	42/42	0.95	0.17	0.90	24,41,79,87	0
15	04C	m	301	42/42	0.94	0.17	0.82	27,42,84,90	0
15	04C	p	301	42/42	0.93	0.18	0.64	25,37,63,75	0
15	04C	4	301	42/42	0.92	0.17	0.62	30,39,54,64	0
15	04C	N	301	42/42	0.94	0.18	0.60	24,34,58,70	0
15	04C	b	301	42/42	0.94	0.17	0.45	28,36,55,65	0
15	04C	x	301	42/42	0.96	0.17	0.29	31,40,52,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	04C	V	301	42/42	0.95	0.16	-0.02	28,40,52,54	0
15	04C	H	301	42/42	0.94	0.14	-0.68	30,37,50,51	0
15	04C	j	301	42/42	0.95	0.15	-0.89	33,37,50,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.