wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 07:11 AM EDT

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

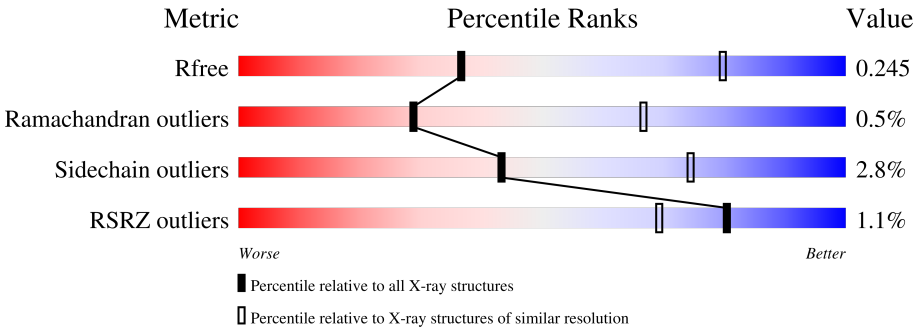
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	96%
1	O	234	2% 96%
1	c	234	95%
1	q	234	94% 6%
2	B	261	92% 5%
2	P	261	92% 5%

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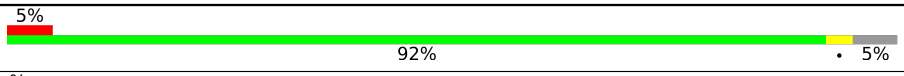
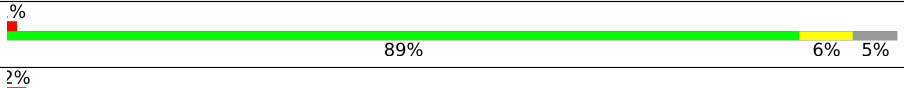
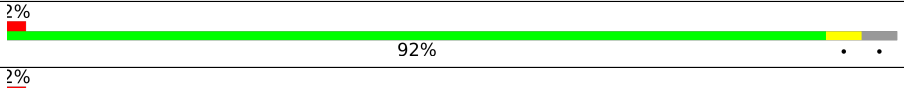
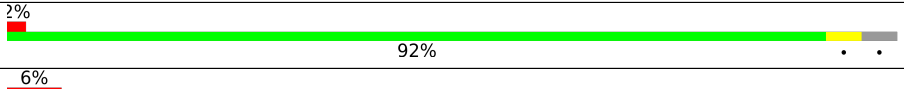
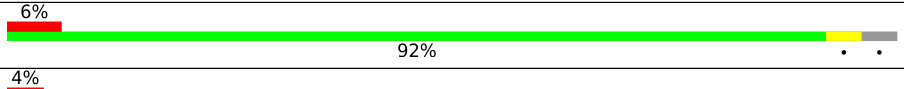
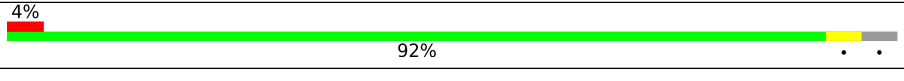
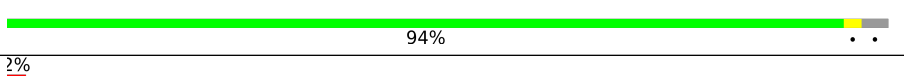
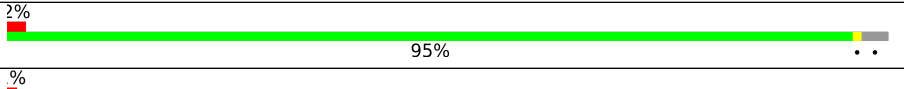
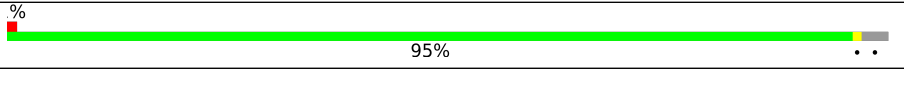
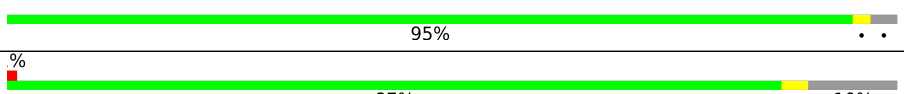
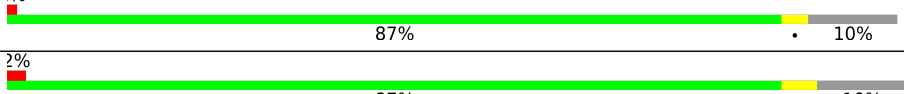
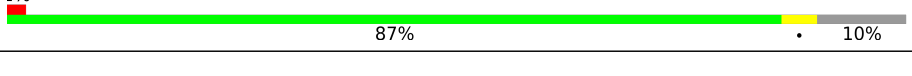
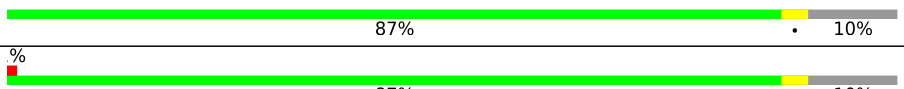
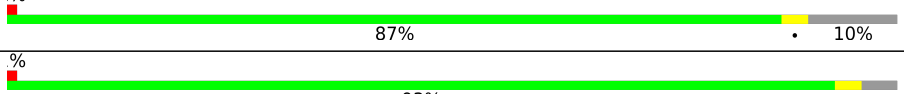
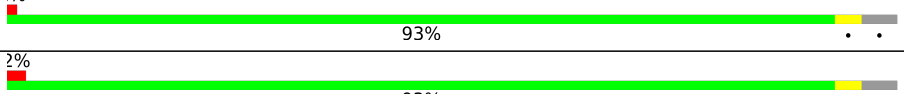
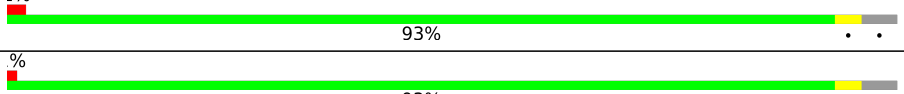
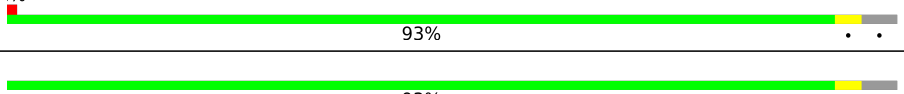
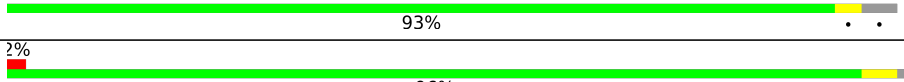
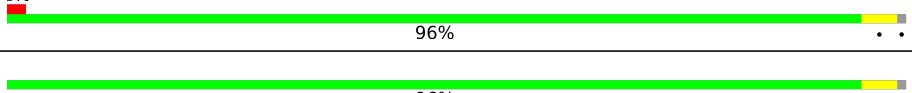
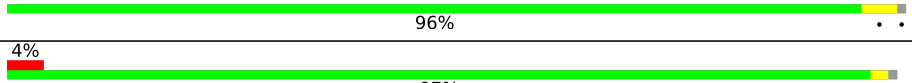
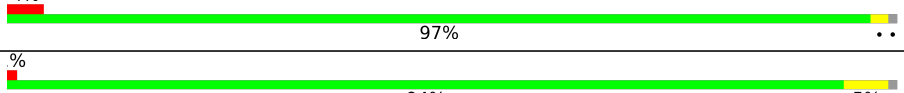
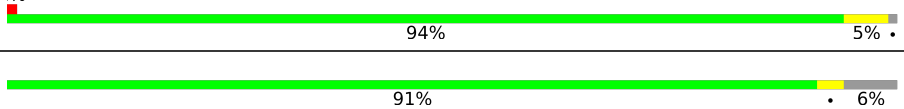
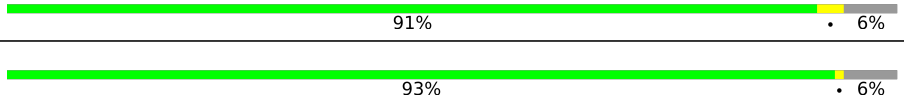
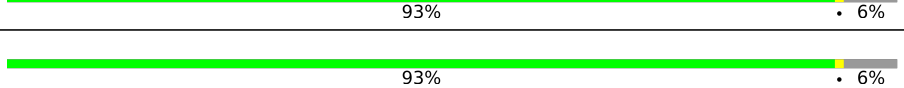
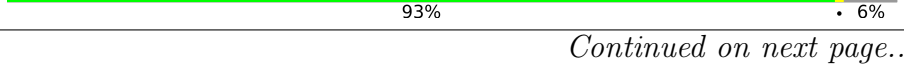
Mol	Chain	Length	Quality of chain
2	d	261	
2	r	261	
3	C	248	
3	Q	248	
3	e	248	
3	s	248	
4	D	241	
4	R	241	
4	f	241	
4	t	241	
5	E	263	
5	S	263	
5	g	263	
5	u	263	
6	F	255	
6	T	255	
6	h	255	
6	v	255	
7	G	246	
7	U	246	
7	i	246	
7	w	246	
8	H	234	
8	V	234	
8	j	234	

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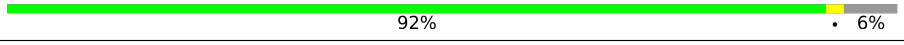
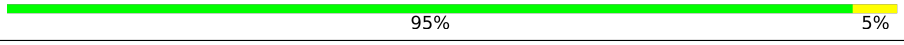
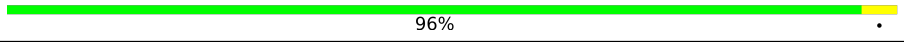
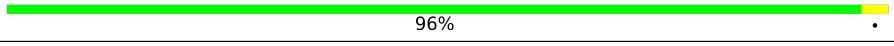
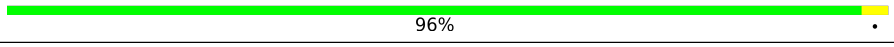
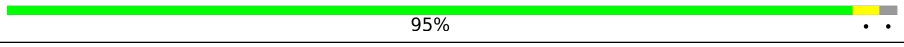
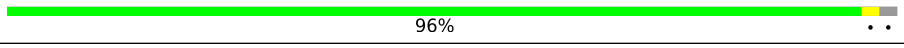
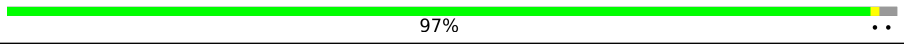
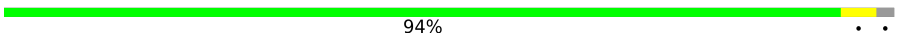
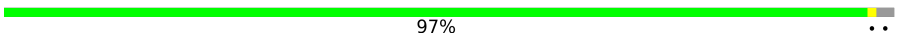
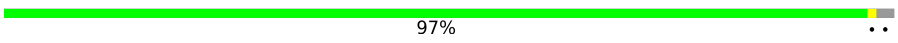
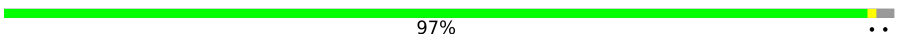
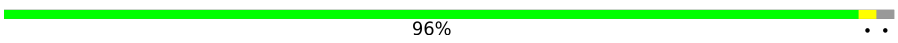
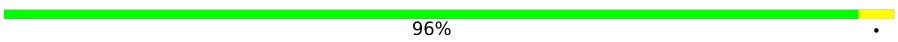
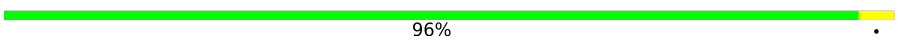
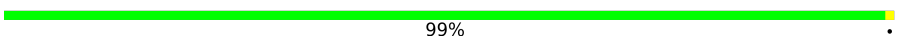
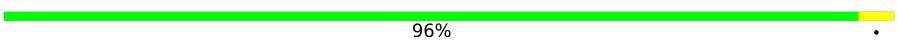
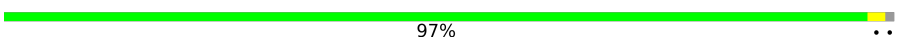
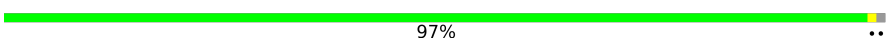
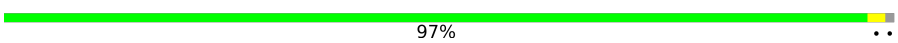
Mol	Chain	Length	Quality of chain
8	x	234	
9	I	205	
9	W	205	
9	k	205	
9	y	205	
10	J	201	
10	X	201	
10	l	201	
10	z	201	
11	1	205	
11	K	205	
11	Y	205	
11	m	205	
12	2	213	
12	L	213	
12	Z	213	
12	n	213	
13	3	219	
13	M	219	
13	a	219	
13	o	219	
14	4	205	
14	N	205	
14	b	205	
14	p	205	

2 Entry composition (i)

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

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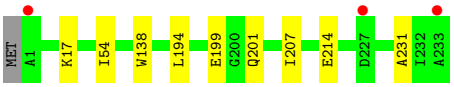
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	n	13	Total O 13 13	0	0
15	o	11	Total O 11 11	0	0
15	p	6	Total O 6 6	0	0
15	q	3	Total O 3 3	0	0
15	r	10	Total O 10 10	0	0
15	s	7	Total O 7 7	0	0
15	t	6	Total O 6 6	0	0
15	u	7	Total O 7 7	0	0
15	v	11	Total O 11 11	0	0
15	w	10	Total O 10 10	0	0
15	x	6	Total O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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

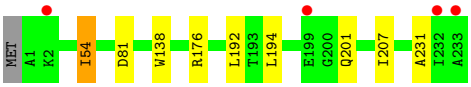
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



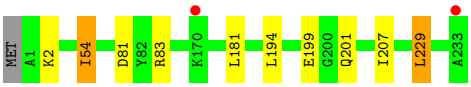
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



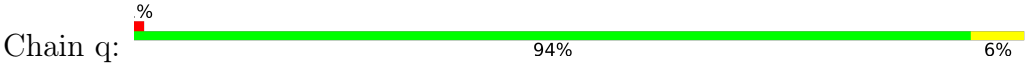
• Molecule 1: Proteasome subunit alpha type-2

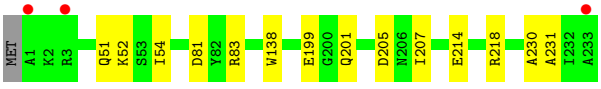
Chain c:



• Molecule 1: Proteasome subunit alpha type-2

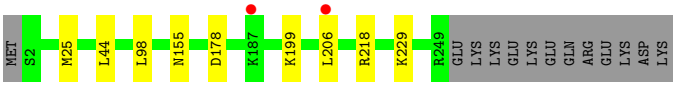
Chain q:





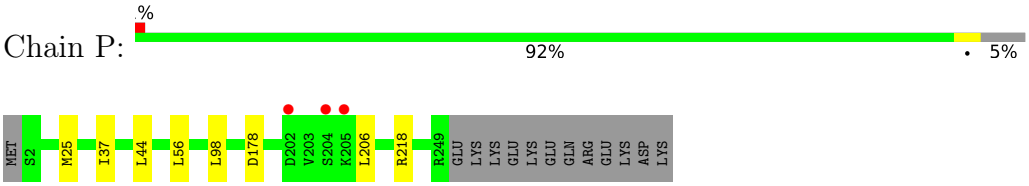
• Molecule 2: Proteasome subunit alpha type-4

Chain B:



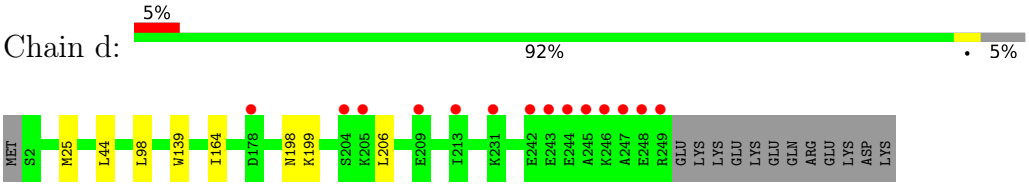
• Molecule 2: Proteasome subunit alpha type-4

Chain P:



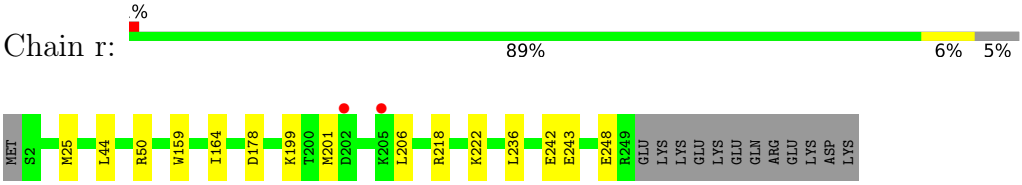
• Molecule 2: Proteasome subunit alpha type-4

Chain d:



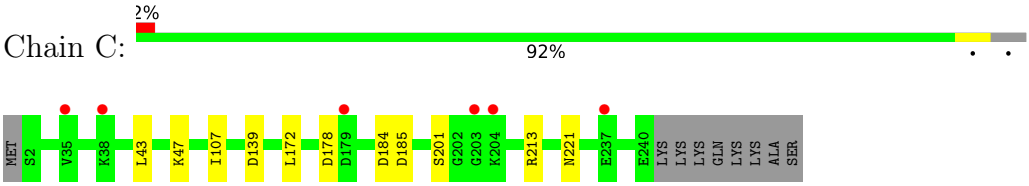
• Molecule 2: Proteasome subunit alpha type-4

Chain r:



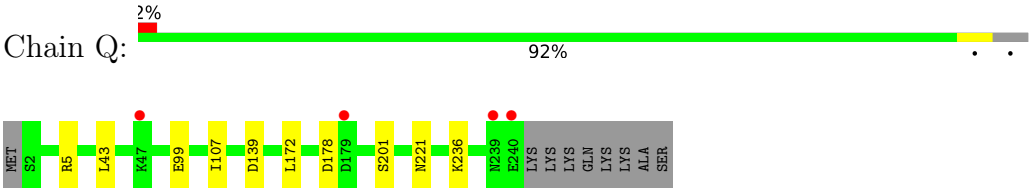
• Molecule 3: Proteasome subunit alpha type-7

Chain C:



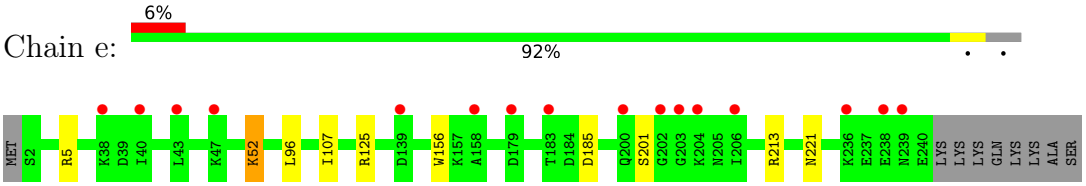
• Molecule 3: Proteasome subunit alpha type-7

Chain Q:



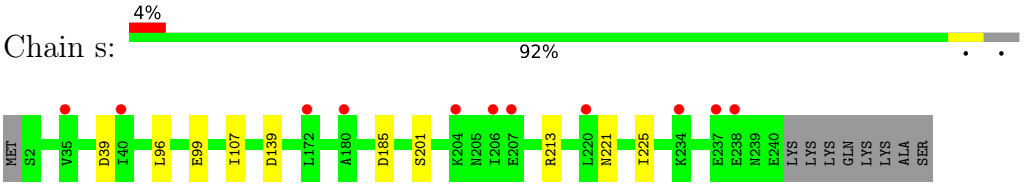
• Molecule 3: Proteasome subunit alpha type-7

Chain e:



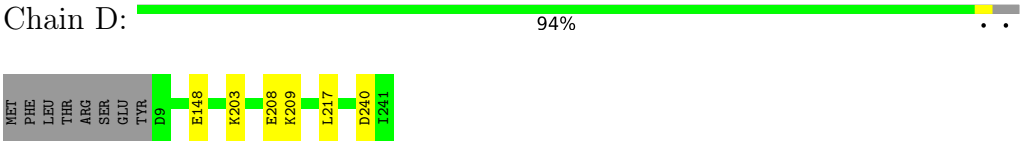
• Molecule 3: Proteasome subunit alpha type-7

Chain s:



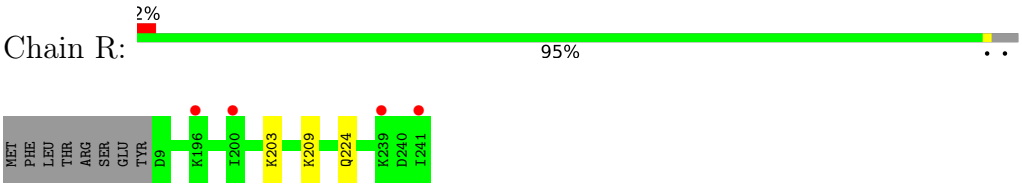
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



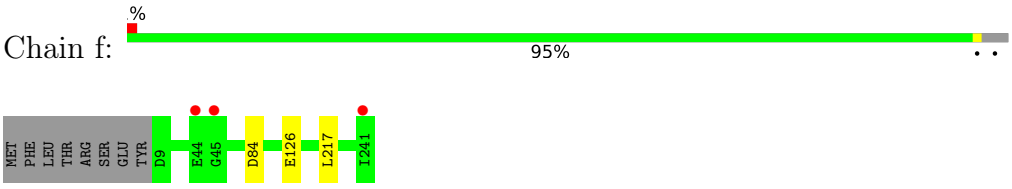
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



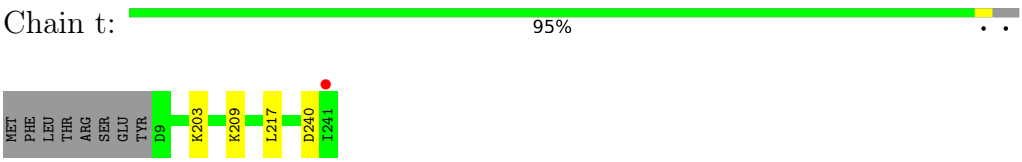
• Molecule 4: Proteasome subunit alpha type-5

Chain f:



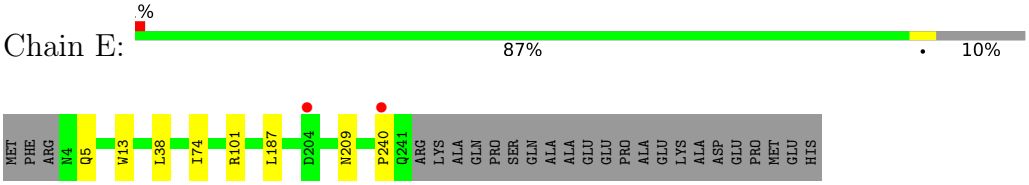
• Molecule 4: Proteasome subunit alpha type-5

Chain t:



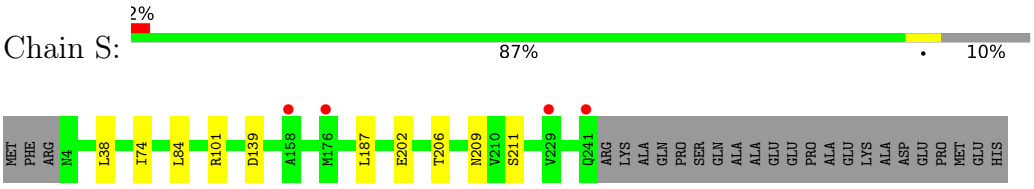
• Molecule 5: Proteasome subunit alpha type-1

Chain E:



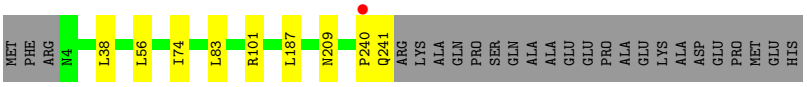
• Molecule 5: Proteasome subunit alpha type-1

Chain S:

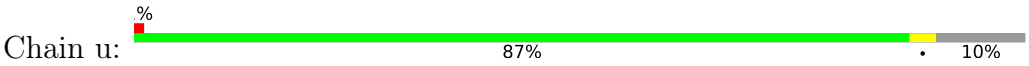


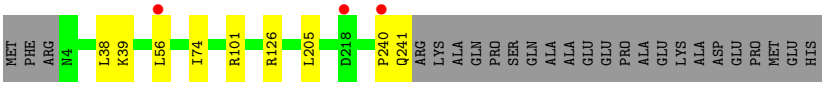
• Molecule 5: Proteasome subunit alpha type-1

Chain g:

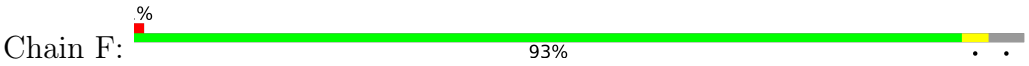


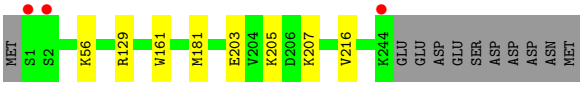
• Molecule 5: Proteasome subunit alpha type-1



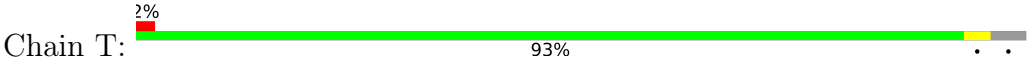


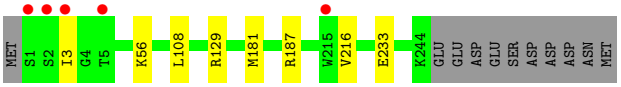
• Molecule 6: Proteasome subunit alpha type-3



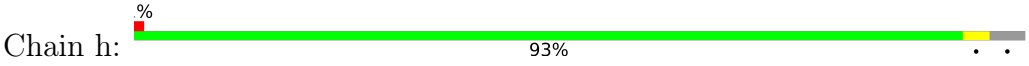


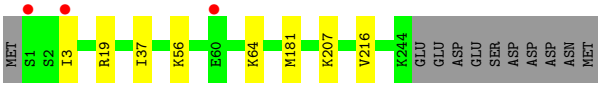
• Molecule 6: Proteasome subunit alpha type-3



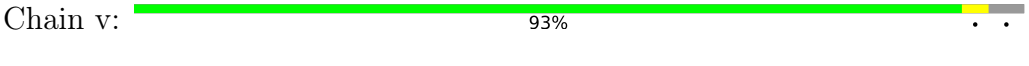


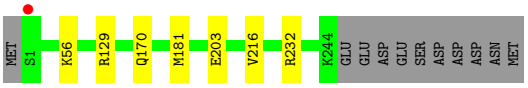
• Molecule 6: Proteasome subunit alpha type-3



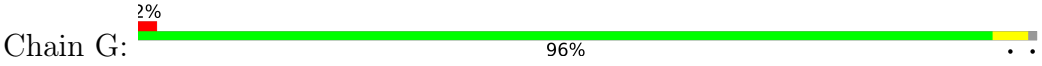


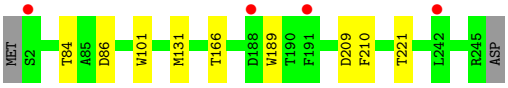
• Molecule 6: Proteasome subunit alpha type-3





• Molecule 7: Proteasome subunit alpha type-6



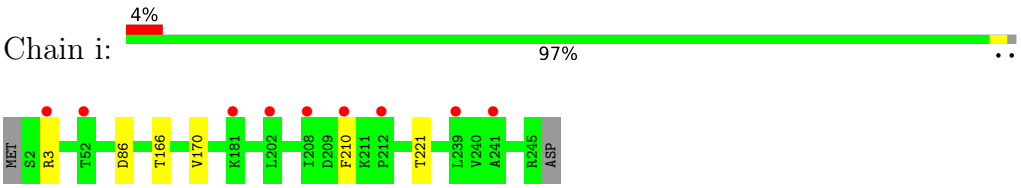


• Molecule 7: Proteasome subunit alpha type-6

Chain U:

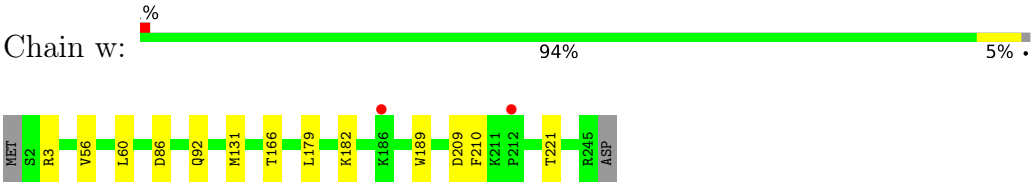
• Molecule 7: Proteasome subunit alpha type-6

Chain i:



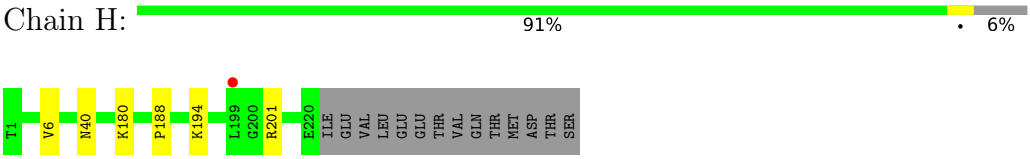
• Molecule 7: Proteasome subunit alpha type-6

Chain w:



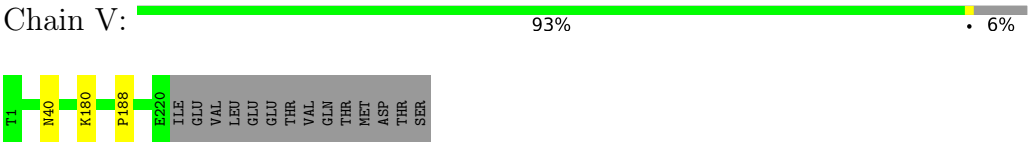
• Molecule 8: Proteasome subunit beta type-7

Chain H:



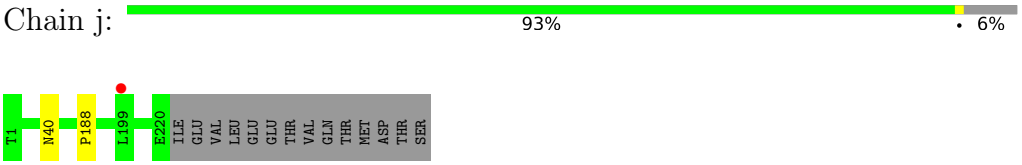
• Molecule 8: Proteasome subunit beta type-7

Chain V:



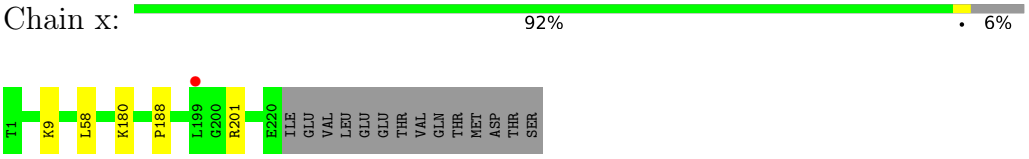
• Molecule 8: Proteasome subunit beta type-7

Chain j:



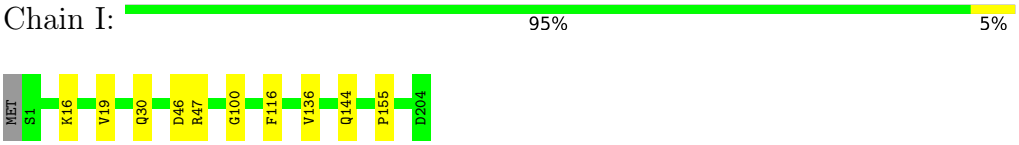
• Molecule 8: Proteasome subunit beta type-7

Chain x:



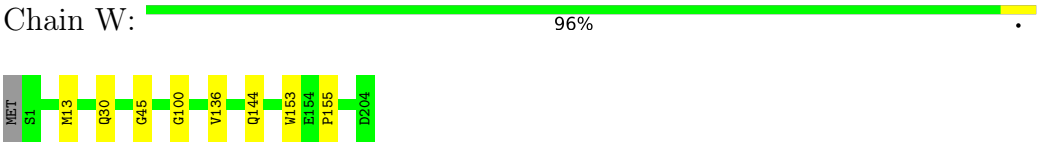
• Molecule 9: Proteasome subunit beta type-3

Chain I:



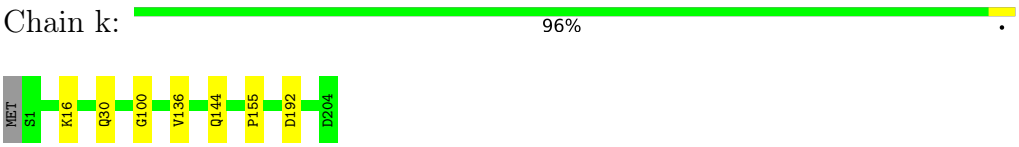
• Molecule 9: Proteasome subunit beta type-3

Chain W:



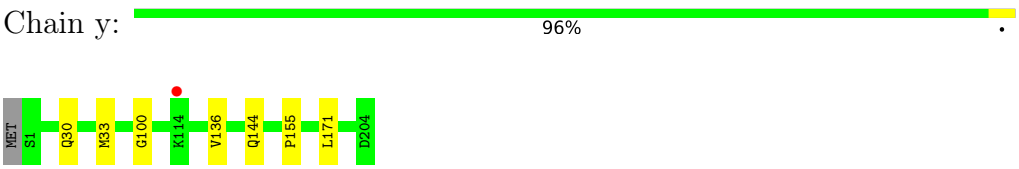
• Molecule 9: Proteasome subunit beta type-3

Chain k:



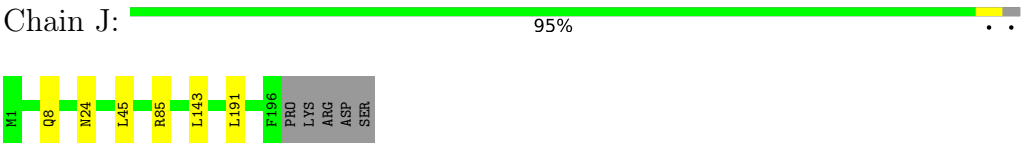
• Molecule 9: Proteasome subunit beta type-3

Chain y:



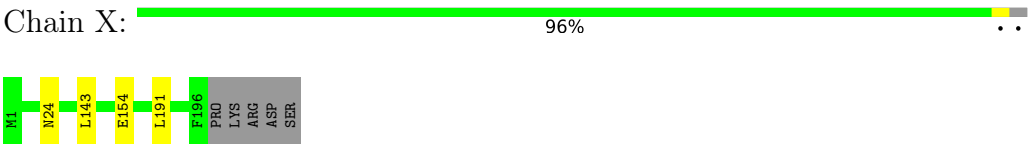
• Molecule 10: Proteasome subunit beta type-2

Chain J:



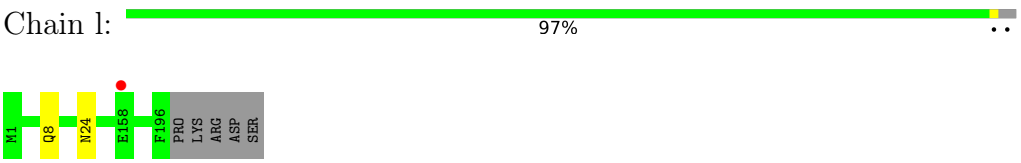
• Molecule 10: Proteasome subunit beta type-2

Chain X:



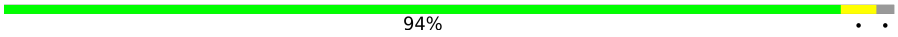
• Molecule 10: Proteasome subunit beta type-2

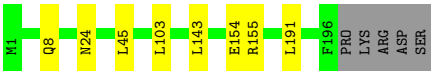
Chain l:



• Molecule 10: Proteasome subunit beta type-2

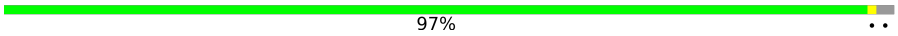
Chain z:

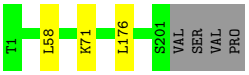




• Molecule 11: Proteasome subunit beta type-5

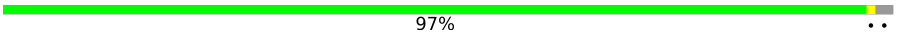
Chain K:

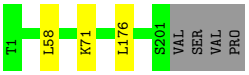




• Molecule 11: Proteasome subunit beta type-5

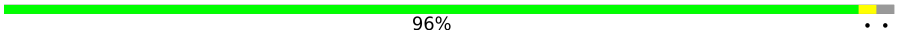
Chain Y:





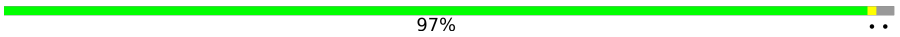
• Molecule 11: Proteasome subunit beta type-5

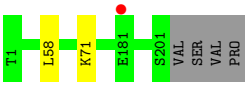
Chain m:



• Molecule 11: Proteasome subunit beta type-5

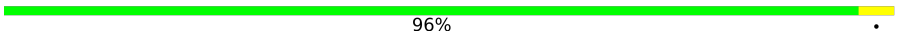
Chain 1:





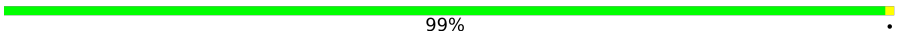
• Molecule 12: Proteasome subunit beta type-1

Chain L:



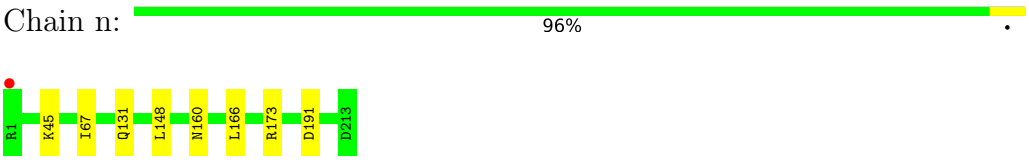
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



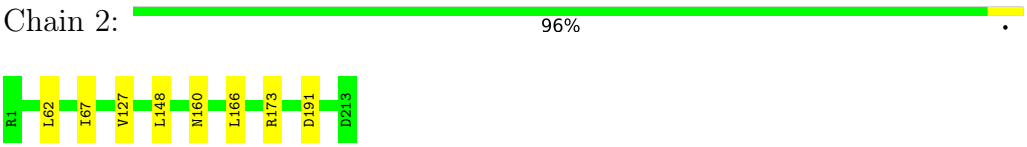
• Molecule 12: Proteasome subunit beta type-1

Chain n:



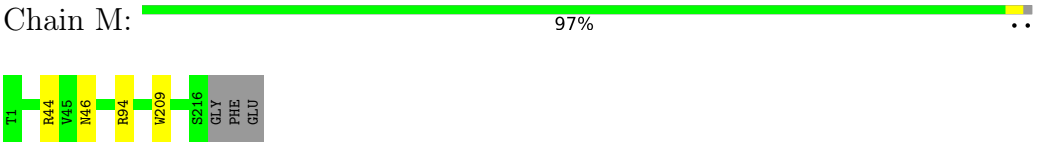
• Molecule 12: Proteasome subunit beta type-1

Chain 2:



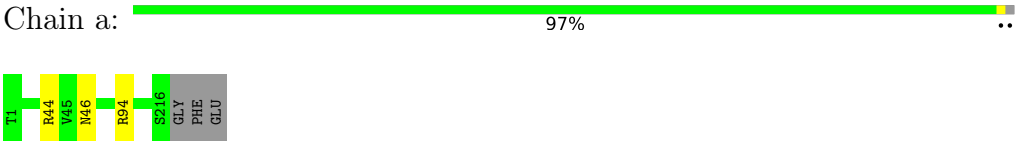
• Molecule 13: Proteasome subunit beta type-4

Chain M:



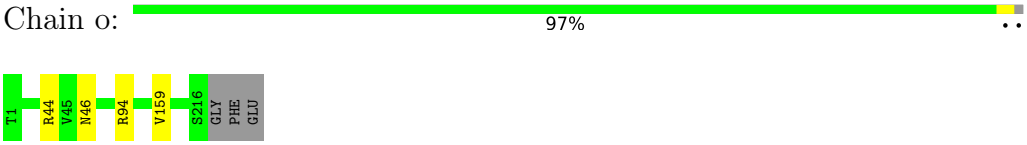
• Molecule 13: Proteasome subunit beta type-4

Chain a:



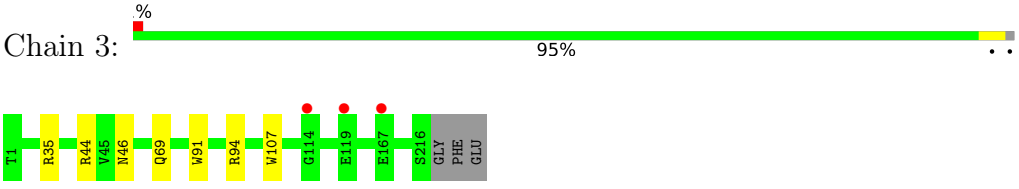
• Molecule 13: Proteasome subunit beta type-4

Chain o:



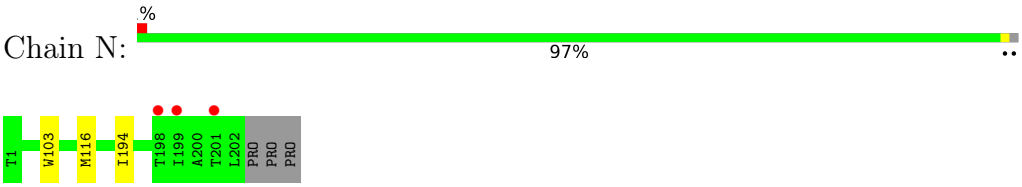
• Molecule 13: Proteasome subunit beta type-4

Chain 3:



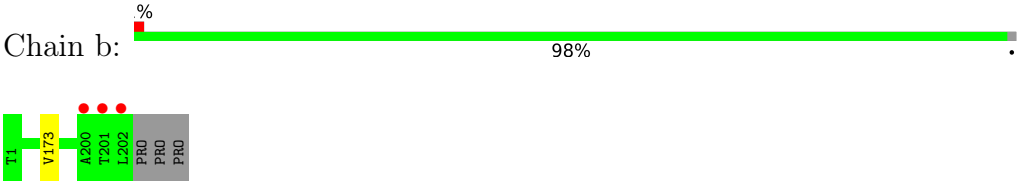
• Molecule 14: Proteasome subunit beta type-6

Chain N:



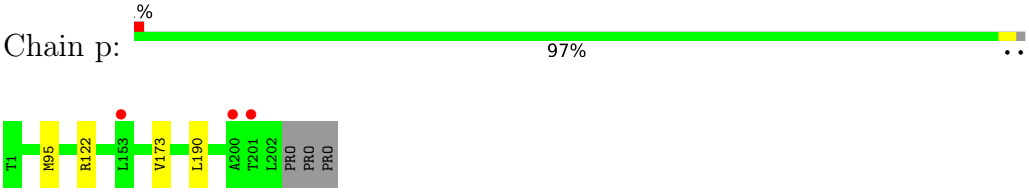
• Molecule 14: Proteasome subunit beta type-6

Chain b:



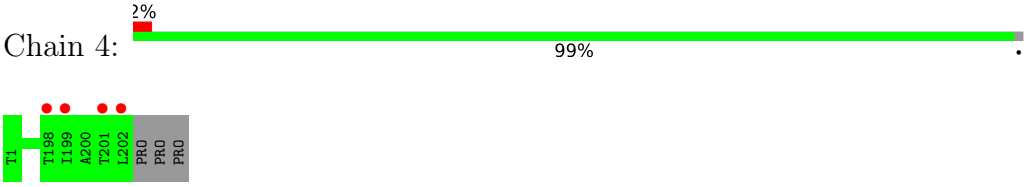
• Molecule 14: Proteasome subunit beta type-6

Chain p:



• Molecule 14: Proteasome subunit beta type-6

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	84.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.38	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	1	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 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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	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%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	12412/12920 (96%)	11795 (95%)	549 (4%)	68 (0%)	29 67

5 of 68 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	189/191 (99%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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

Mol	Chain	Res	Type
3	s	107	ILE
12	2	148	LEU
4	t	209	LYS
7	w	166	THR
4	R	209	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
12	Z	146	GLN
10	z	8	GLN
7	i	127	GLN
9	y	144	GLN
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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	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^2)	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, 172	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^2)	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

The worst 5 of 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

6.2 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.