



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:11 am GMT

PDB ID : 4R3O  
Title : Human Constitutive 20S Proteasome  
Authors : Sacchettini, J.C.; Harshbarger, W.H.  
Deposited on : 2014-08-16  
Resolution : 2.60 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

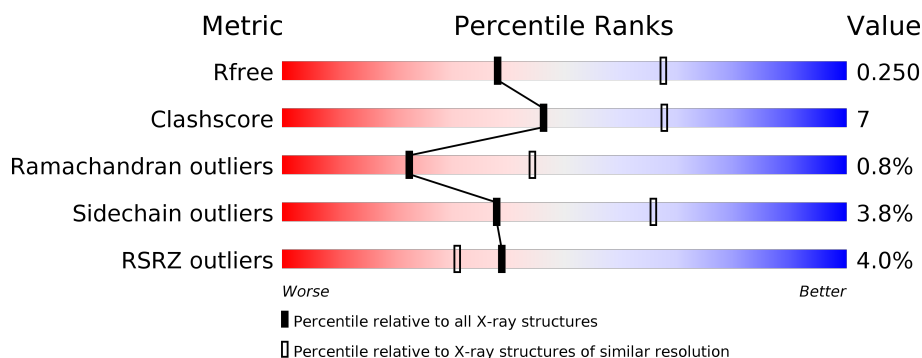
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	244	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	O	244	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
2	B	233	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
2	P	233	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
3	C	250	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
3	Q	250	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	243	
4	R	243	
5	E	234	
5	S	234	
6	F	238	
6	T	238	
7	G	245	
7	U	245	
8	H	202	
8	V	202	
9	I	220	
9	W	220	
10	J	204	
10	X	204	
11	K	199	
11	Y	199	
12	L	201	
12	Z	201	
13	1	213	
13	M	213	
14	2	217	
14	N	217	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47831 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			
1	O	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1707	1081	287	334	5			
2	P	233	Total	C	N	O	S	0	0	0
			1712	1085	287	334	6			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			1912	1204	329	371	8			
3	Q	250	Total	C	N	O	S	0	0	0
			1913	1203	330	372	8			

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1724	1068	312	339	5			
4	R	243	Total	C	N	O	S	0	0	0
			1691	1051	309	327	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	S	234	Total	C	N	O	S	0	0	0
			1716	1102	290	313	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	T	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	U	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	V	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	W	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	Y	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	Z	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1641	1036	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1644	1039	282	313	10			

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1676	1057	287	320	12			
14	2	217	Total	C	N	O	S	0	0	0
			1678	1058	290	318	12			

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	O	0	0
			2	2		
15	D	4	Total	O	0	0
			4	4		

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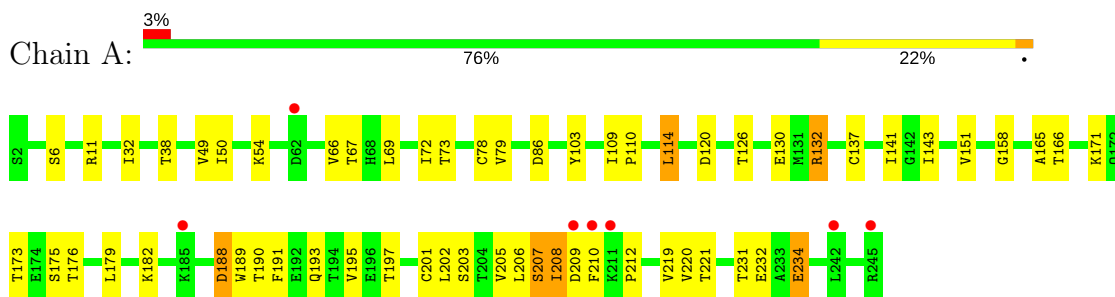
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	E	8	Total 8	O 8	0	0
15	F	19	Total 19	O 19	0	0
15	G	1	Total 1	O 1	0	0
15	K	9	Total 9	O 9	0	0
15	L	8	Total 8	O 8	0	0
15	M	34	Total 34	O 34	0	0
15	N	11	Total 11	O 11	0	0
15	O	1	Total 1	O 1	0	0
15	P	24	Total 24	O 24	0	0
15	Q	10	Total 10	O 10	0	0
15	R	5	Total 5	O 5	0	0
15	W	17	Total 17	O 17	0	0
15	X	25	Total 25	O 25	0	0
15	Y	3	Total 3	O 3	0	0
15	Z	4	Total 4	O 4	0	0

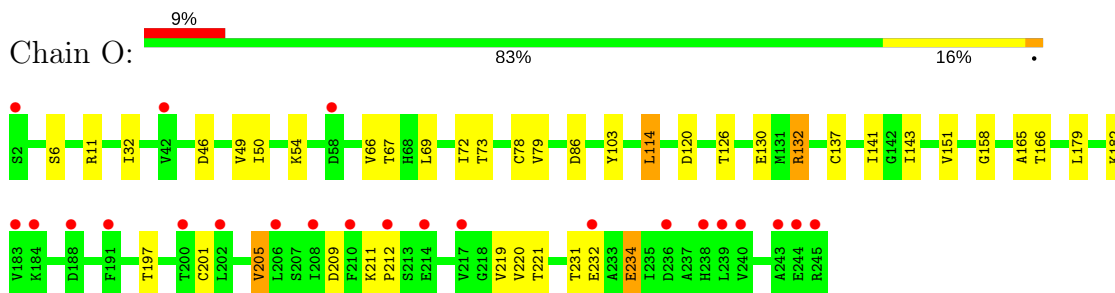
### 3 Residue-property plots [i](#)

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

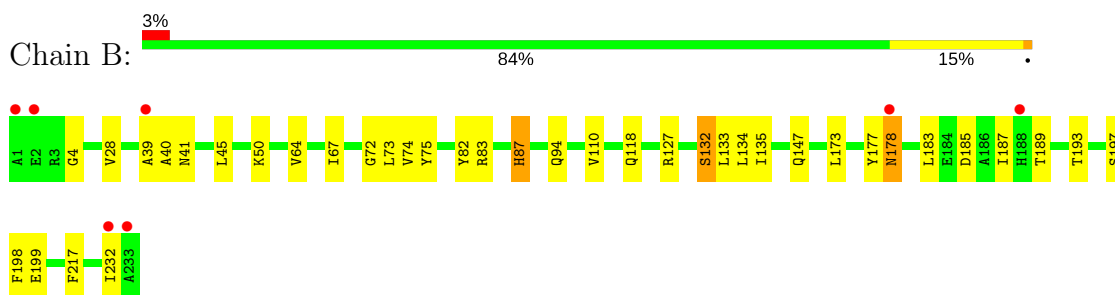
- Molecule 1: Proteasome subunit alpha type-6



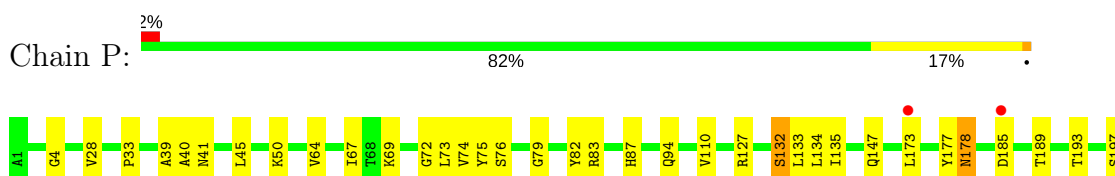
- Molecule 1: Proteasome subunit alpha type-6



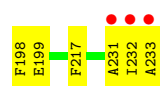
- Molecule 2: Proteasome subunit alpha type-2



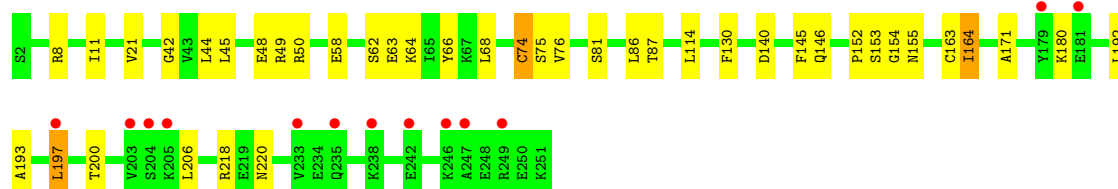
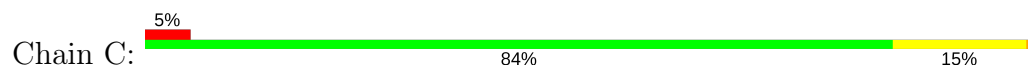
- Molecule 2: Proteasome subunit alpha type-2



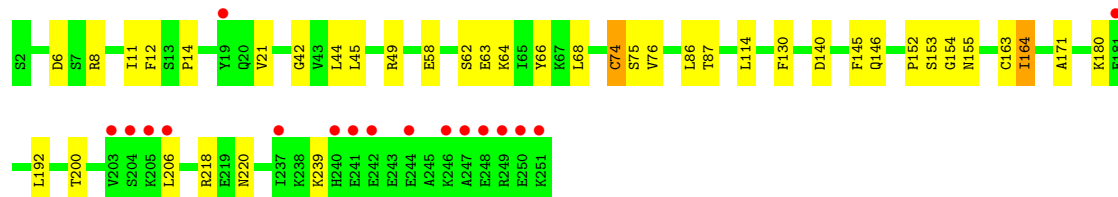
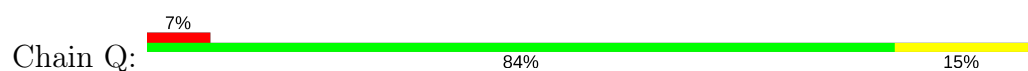




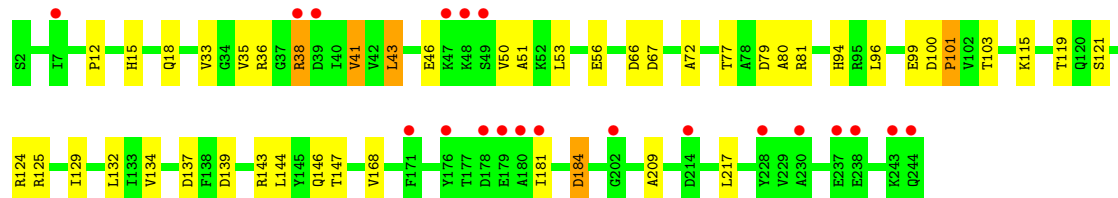
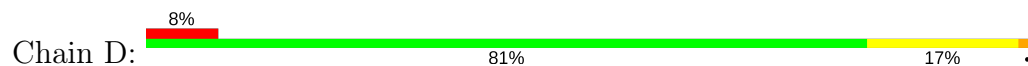
• Molecule 3: Proteasome subunit alpha type-4



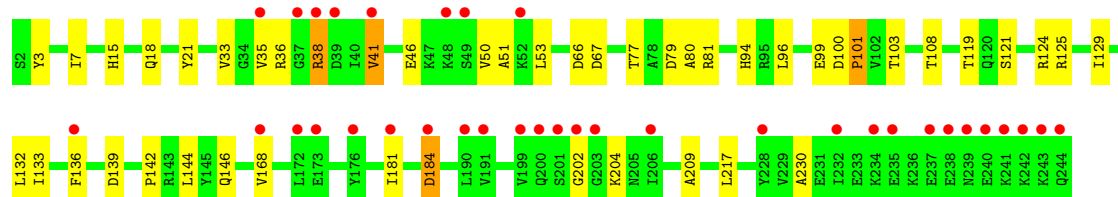
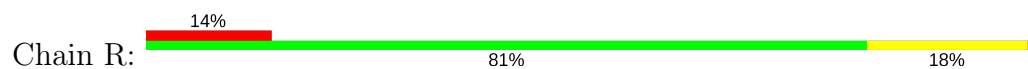
• Molecule 3: Proteasome subunit alpha type-4



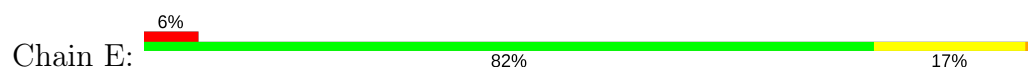
• Molecule 4: Proteasome subunit alpha type-7

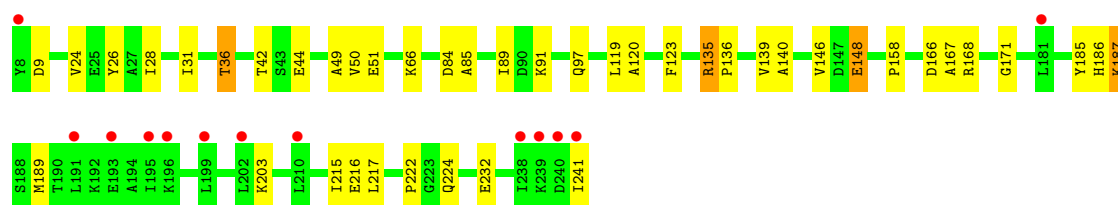


• Molecule 4: Proteasome subunit alpha type-7

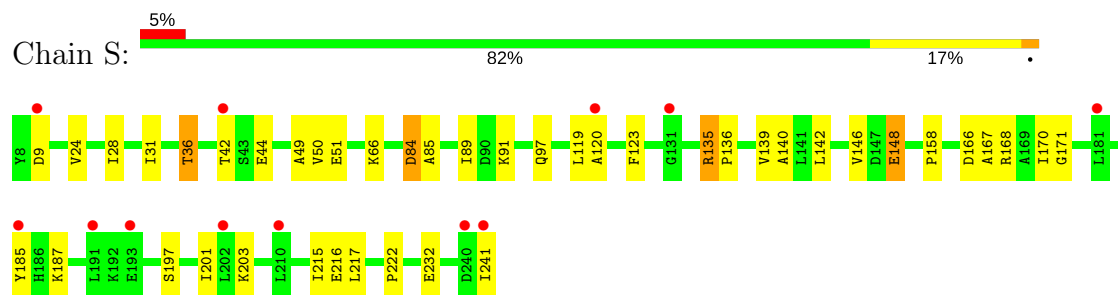


• Molecule 5: Proteasome subunit alpha type-5

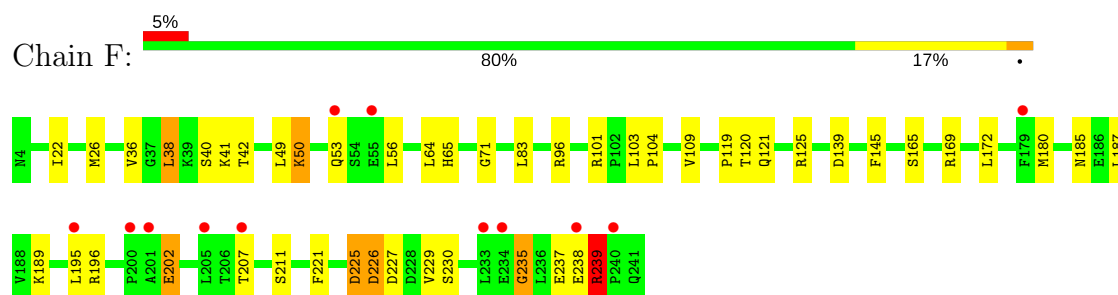




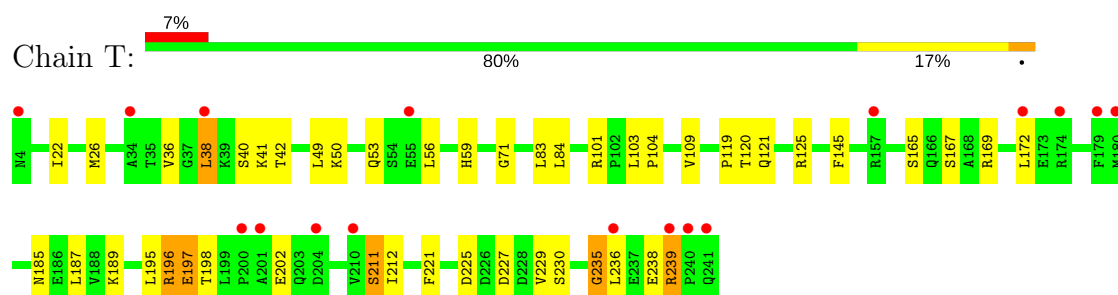
- Molecule 5: Proteasome subunit alpha type-5



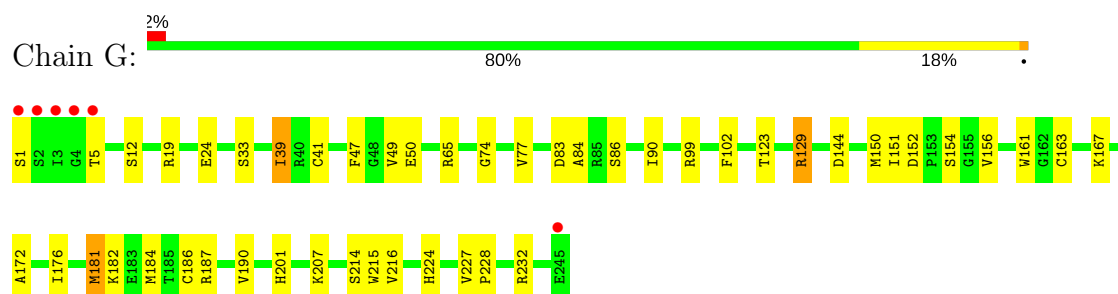
- Molecule 6: Proteasome subunit alpha type-1



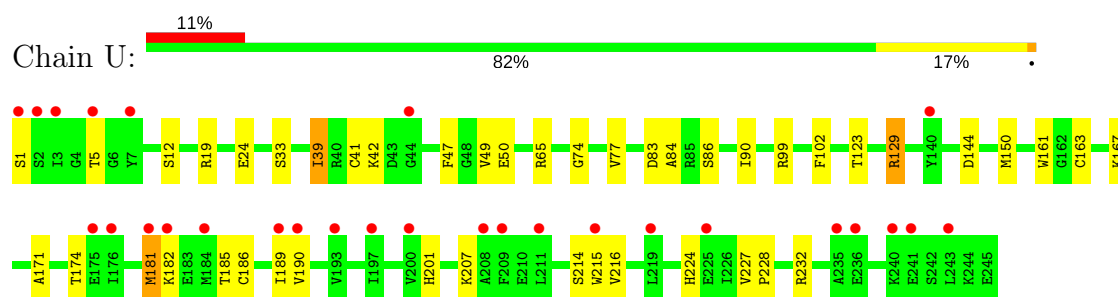
- Molecule 6: Proteasome subunit alpha type-1



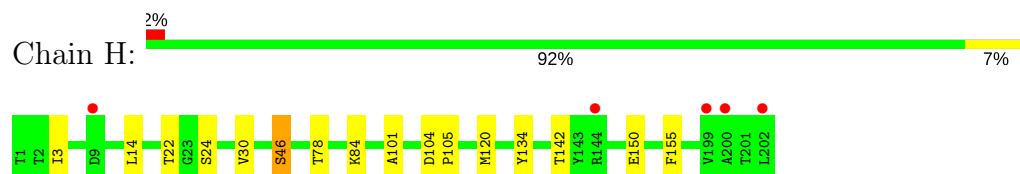
- Molecule 7: Proteasome subunit alpha type-3



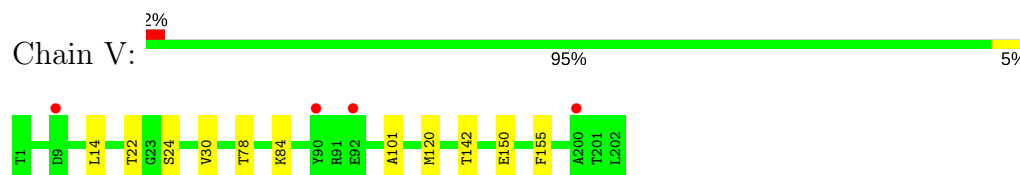
- Molecule 7: Proteasome subunit alpha type-3



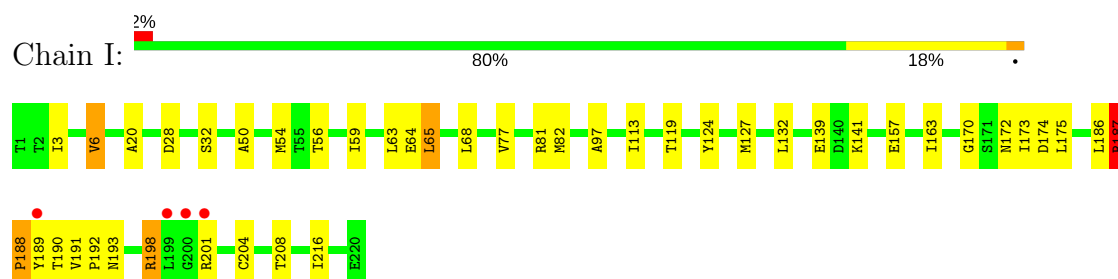
• Molecule 8: Proteasome subunit beta type-6



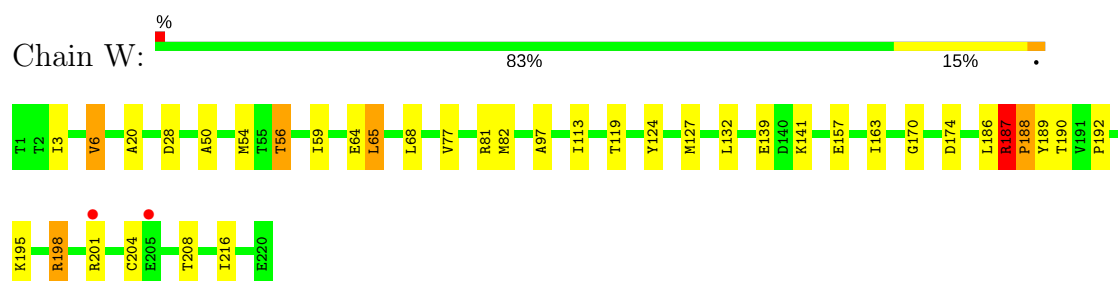
• Molecule 8: Proteasome subunit beta type-6



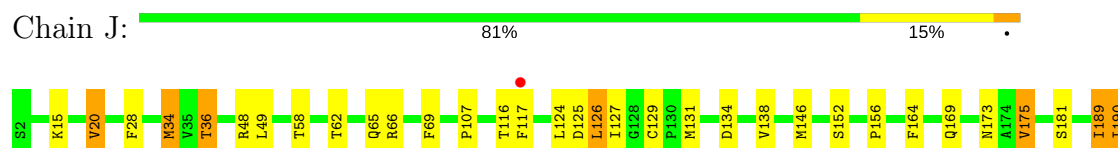
• Molecule 9: Proteasome subunit beta type-7



• Molecule 9: Proteasome subunit beta type-7



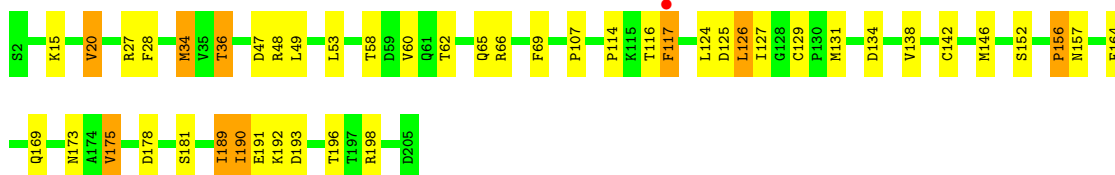
• Molecule 10: Proteasome subunit beta type-3





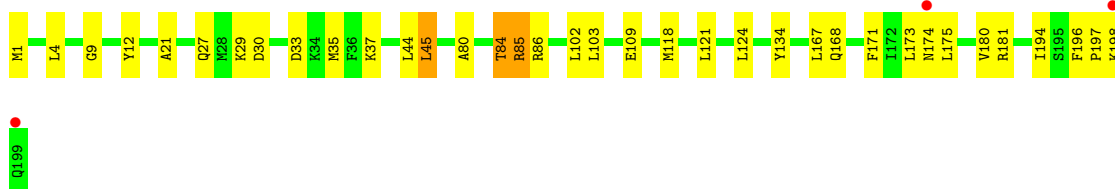
• Molecule 10: Proteasome subunit beta type-3

Chain X: 77% 18% .



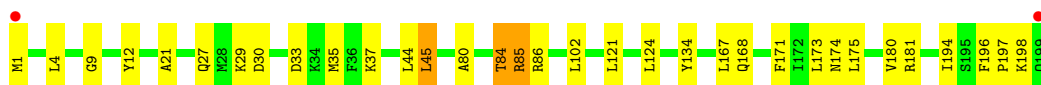
• Molecule 11: Proteasome subunit beta type-2

Chain K: 2% 82% 17% .



• Molecule 11: Proteasome subunit beta type-2

Chain Y: 83% 15% .



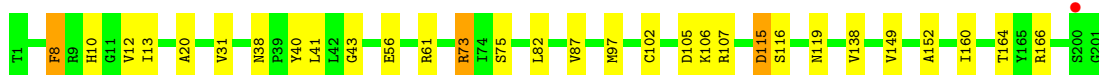
• Molecule 12: Proteasome subunit beta type-5

Chain L: 82% 17% .

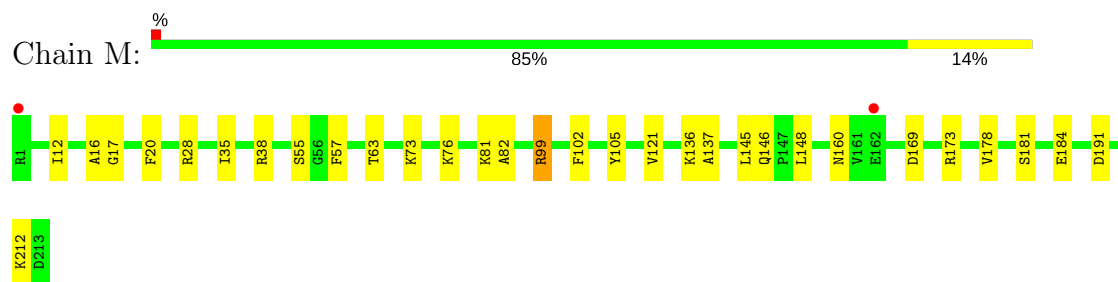


• Molecule 12: Proteasome subunit beta type-5

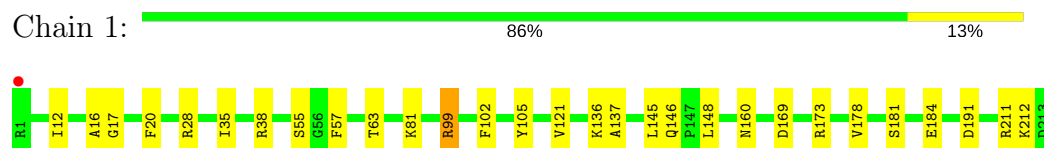
Chain Z: 85% 13% .



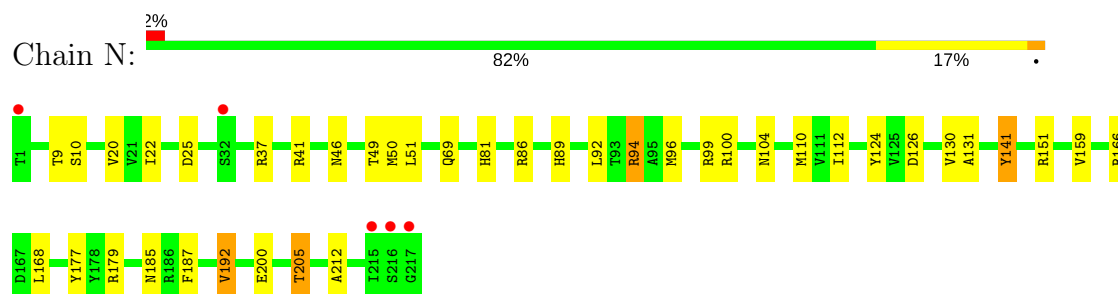
• Molecule 13: Proteasome subunit beta type-1



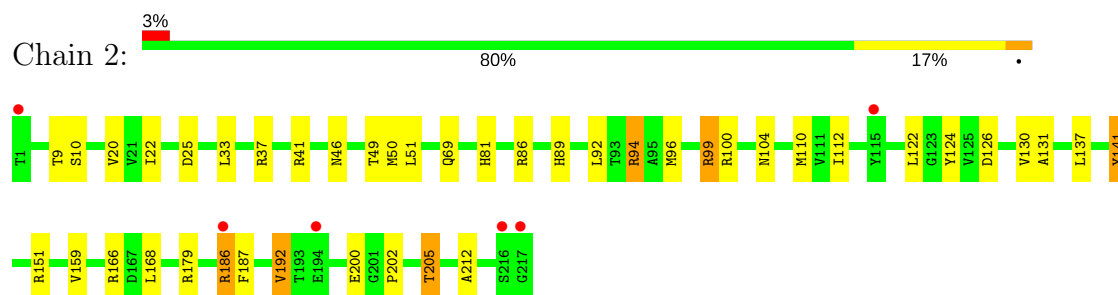
- Molecule 13: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.23Å 205.06Å 163.13Å 90.00° 106.37° 90.00°	Depositor
Resolution (Å)	36.34 – 2.60 49.42 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.34-2.60) 87.9 (49.42-2.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.204 , 0.244 0.215 , 0.250	Depositor DCC
$R_{free}$ test set	11374 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	47831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/1878	0.45	0/2549
1	O	0.24	0/1878	0.42	0/2549
2	B	0.25	0/1742	0.42	0/2372
2	P	0.25	0/1747	0.43	0/2378
3	C	0.24	0/1942	0.43	0/2628
3	Q	0.24	0/1943	0.43	0/2629
4	D	0.23	0/1748	0.44	0/2386
4	R	0.23	0/1716	0.44	0/2347
5	E	0.25	0/1786	0.42	0/2419
5	S	0.24	0/1743	0.42	0/2333
6	F	0.29	0/1885	0.46	1/2552 (0.0%)
6	T	0.25	0/1885	0.44	0/2552
7	G	0.26	0/1920	0.42	0/2591
7	U	0.27	0/1920	0.44	0/2591
8	H	0.27	0/1535	0.43	0/2078
8	V	0.26	0/1535	0.44	0/2078
9	I	0.32	1/1670 (0.1%)	0.49	1/2265 (0.0%)
9	W	0.28	0/1670	0.45	0/2265
10	J	0.26	0/1614	0.45	0/2177
10	X	0.26	0/1614	0.45	0/2177
11	K	0.24	0/1603	0.44	0/2174
11	Y	0.25	0/1603	0.44	0/2174
12	L	0.28	0/1579	0.45	0/2134
12	Z	0.25	0/1582	0.45	0/2138
13	1	0.28	0/1674	0.45	0/2257
13	M	0.31	0/1671	0.46	0/2253
14	2	0.25	0/1711	0.44	0/2319
14	N	0.25	0/1709	0.44	0/2317
All	All	0.26	1/48503 (0.0%)	0.44	2/65682 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	188	PRO	N-CD	5.13	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	239	ARG	C-N-CD	6.04	141.09	128.40
9	I	187	ARG	C-N-CD	5.11	139.14	128.40

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1845	0	1805	52	0
1	O	1845	0	1805	27	0
2	B	1707	0	1591	25	0
2	P	1712	0	1605	33	0
3	C	1912	0	1851	21	0
3	Q	1913	0	1848	23	0
4	D	1724	0	1525	25	0
4	R	1691	0	1468	27	0
5	E	1759	0	1707	32	0
5	S	1716	0	1707	25	0
6	F	1850	0	1822	46	0
6	T	1850	0	1822	42	0
7	G	1885	0	1845	28	0
7	U	1885	0	1845	28	0
8	H	1509	0	1473	12	0
8	V	1509	0	1473	10	0
9	I	1643	0	1644	40	0
9	W	1643	0	1644	34	0
10	J	1585	0	1598	24	0
10	X	1585	0	1598	29	0
11	K	1570	0	1547	23	0
11	Y	1570	0	1547	21	0
12	L	1548	0	1499	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1551	0	1508	19	0
13	1	1644	0	1627	20	0
13	M	1641	0	1618	26	0
14	2	1678	0	1640	28	0
14	N	1676	0	1633	29	0
15	A	2	0	0	0	0
15	D	4	0	0	0	0
15	E	8	0	0	6	0
15	F	19	0	0	9	0
15	G	1	0	0	0	0
15	K	9	0	0	1	0
15	L	8	0	0	1	0
15	M	34	0	0	3	0
15	N	11	0	0	0	0
15	O	1	0	0	0	0
15	P	24	0	0	10	0
15	Q	10	0	0	1	0
15	R	5	0	0	2	0
15	W	17	0	0	1	0
15	X	25	0	0	3	0
15	Y	3	0	0	0	0
15	Z	4	0	0	0	0
All	All	47831	0	46295	680	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 7.

The worst 5 of 680 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)
9:W:187:ARG:HB3	9:W:188:PRO:CD	1.57	1.28
9:W:187:ARG:HB3	9:W:188:PRO:HD2	1.13	1.11
9:W:187:ARG:CB	9:W:188:PRO:CD	2.35	1.05
6:T:196:ARG:HD3	6:T:239:ARG:HE	1.21	1.03
6:F:189:LYS:HD3	15:F:317:HOH:O	1.63	0.99

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	230 (95%)	7 (3%)	5 (2%)	8	15
1	O	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	38	63
2	B	231/233 (99%)	210 (91%)	18 (8%)	3 (1%)	14	29
2	P	231/233 (99%)	209 (90%)	19 (8%)	3 (1%)	14	29
3	C	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	38	63
3	Q	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	38	63
4	D	241/243 (99%)	222 (92%)	16 (7%)	3 (1%)	15	32
4	R	241/243 (99%)	222 (92%)	15 (6%)	4 (2%)	11	21
5	E	232/234 (99%)	220 (95%)	10 (4%)	2 (1%)	20	40
5	S	232/234 (99%)	220 (95%)	10 (4%)	2 (1%)	20	40
6	F	236/238 (99%)	223 (94%)	9 (4%)	4 (2%)	11	21
6	T	236/238 (99%)	224 (95%)	9 (4%)	3 (1%)	14	29
7	G	243/245 (99%)	233 (96%)	8 (3%)	2 (1%)	22	44
7	U	243/245 (99%)	234 (96%)	7 (3%)	2 (1%)	22	44
8	H	200/202 (99%)	196 (98%)	4 (2%)	0	100	100
8	V	200/202 (99%)	196 (98%)	4 (2%)	0	100	100
9	I	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
9	W	218/220 (99%)	208 (95%)	8 (4%)	2 (1%)	20	40
10	J	202/204 (99%)	189 (94%)	11 (5%)	2 (1%)	18	37
10	X	202/204 (99%)	189 (94%)	11 (5%)	2 (1%)	18	37
11	K	197/199 (99%)	188 (95%)	7 (4%)	2 (1%)	18	37
11	Y	197/199 (99%)	188 (95%)	7 (4%)	2 (1%)	18	37
12	L	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
12	Z	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
13	1	211/213 (99%)	204 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
14	2	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	32	58
14	N	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	32	58
All	All	6230/6286 (99%)	5913 (95%)	269 (4%)	48 (1%)	22	44

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	PRO
5	E	120	ALA
6	F	238	GLU
7	G	207	LYS
10	J	156	PRO

### 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	193/208 (93%)	185 (96%)	8 (4%)	35	63
1	O	193/208 (93%)	184 (95%)	9 (5%)	30	57
2	B	163/190 (86%)	160 (98%)	3 (2%)	64	85
2	P	165/190 (87%)	162 (98%)	3 (2%)	64	85
3	C	193/210 (92%)	184 (95%)	9 (5%)	30	57
3	Q	193/210 (92%)	185 (96%)	8 (4%)	35	63
4	D	152/207 (73%)	141 (93%)	11 (7%)	17	33
4	R	142/207 (69%)	133 (94%)	9 (6%)	21	42
5	E	189/196 (96%)	185 (98%)	4 (2%)	59	83
5	S	189/196 (96%)	184 (97%)	5 (3%)	51	78
6	F	198/204 (97%)	192 (97%)	6 (3%)	46	74
6	T	198/204 (97%)	190 (96%)	8 (4%)	36	64
7	G	195/202 (96%)	189 (97%)	6 (3%)	45	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	195/202 (96%)	188 (96%)	7 (4%)	40	68
8	H	155/157 (99%)	152 (98%)	3 (2%)	62	84
8	V	155/157 (99%)	153 (99%)	2 (1%)	73	90
9	I	177/181 (98%)	168 (95%)	9 (5%)	28	52
9	W	177/181 (98%)	169 (96%)	8 (4%)	32	59
10	J	172/173 (99%)	162 (94%)	10 (6%)	23	46
10	X	172/173 (99%)	161 (94%)	11 (6%)	20	40
11	K	164/170 (96%)	159 (97%)	5 (3%)	46	74
11	Y	164/170 (96%)	159 (97%)	5 (3%)	46	74
12	L	153/156 (98%)	148 (97%)	5 (3%)	43	70
12	Z	154/156 (99%)	148 (96%)	6 (4%)	37	65
13	1	175/178 (98%)	174 (99%)	1 (1%)	89	96
13	M	174/178 (98%)	172 (99%)	2 (1%)	78	92
14	2	175/179 (98%)	163 (93%)	12 (7%)	18	36
14	N	175/179 (98%)	165 (94%)	10 (6%)	24	47
All	All	4900/5222 (94%)	4715 (96%)	185 (4%)	38	66

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	86	ARG
3	Q	44	LEU
12	Z	115	ASP
14	N	141	TYR
1	O	114	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
12	Z	10	HIS
14	2	81	HIS
12	Z	38	ASN
13	M	146	GLN
13	1	146	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	244/244 (100%)	0.13	7 (2%)	52	45	55, 89, 135, 176	0
1	O	244/244 (100%)	0.43	23 (9%)	9	6	57, 97, 148, 214	0
2	B	233/233 (100%)	0.12	7 (3%)	51	43	56, 83, 130, 210	0
2	P	233/233 (100%)	0.20	5 (2%)	64	58	57, 83, 129, 215	0
3	C	250/250 (100%)	0.21	13 (5%)	28	21	57, 87, 147, 232	0
3	Q	250/250 (100%)	0.34	17 (6%)	18	13	54, 89, 157, 228	0
4	D	243/243 (100%)	0.42	20 (8%)	12	8	55, 95, 177, 238	0
4	R	243/243 (100%)	0.61	35 (14%)	3	1	53, 98, 190, 261	0
5	E	234/234 (100%)	0.27	13 (5%)	25	19	51, 90, 134, 187	0
5	S	234/234 (100%)	0.30	12 (5%)	29	22	50, 91, 134, 178	0
6	F	238/238 (100%)	0.31	12 (5%)	30	23	50, 79, 125, 199	0
6	T	238/238 (100%)	0.33	17 (7%)	17	12	54, 82, 130, 246	0
7	G	245/245 (100%)	0.20	6 (2%)	59	52	59, 85, 131, 198	0
7	U	245/245 (100%)	0.59	28 (11%)	6	3	61, 92, 145, 222	0
8	H	202/202 (100%)	0.16	5 (2%)	58	50	53, 69, 111, 212	0
8	V	202/202 (100%)	0.16	4 (1%)	65	59	50, 70, 113, 171	0
9	I	220/220 (100%)	0.09	4 (1%)	69	63	51, 67, 109, 169	0
9	W	220/220 (100%)	0.07	2 (0%)	84	81	48, 67, 114, 157	0
10	J	204/204 (100%)	0.04	1 (0%)	90	89	47, 66, 99, 150	0
10	X	204/204 (100%)	0.00	1 (0%)	90	89	46, 65, 96, 141	0
11	K	199/199 (100%)	0.06	3 (1%)	74	69	47, 70, 103, 207	0
11	Y	199/199 (100%)	0.09	2 (1%)	82	79	49, 70, 101, 171	0
12	L	201/201 (100%)	0.02	1 (0%)	90	89	41, 66, 100, 140	0
12	Z	201/201 (100%)	-0.08	1 (0%)	90	89	46, 66, 101, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1	213/213 (100%)	-0.10	1 (0%) 90 89	42, 63, 92, 149	0
13	M	213/213 (100%)	-0.06	2 (0%) 84 81	44, 61, 94, 137	0
14	2	217/217 (100%)	0.07	6 (2%) 53 46	42, 69, 101, 167	0
14	N	217/217 (100%)	0.12	5 (2%) 61 54	42, 64, 102, 192	0
All	All	6286/6286 (100%)	0.19	253 (4%) 39 31	41, 77, 135, 261	0

The worst 5 of 253 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	233	ALA	17.0
2	P	232	ILE	13.8
11	K	199	GLN	13.6
2	B	233	ALA	12.7
6	T	240	PRO	12.6

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.