



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:46 PM GMT

PDB ID : 3UNH
Title : Mouse 20S immunoproteasome
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

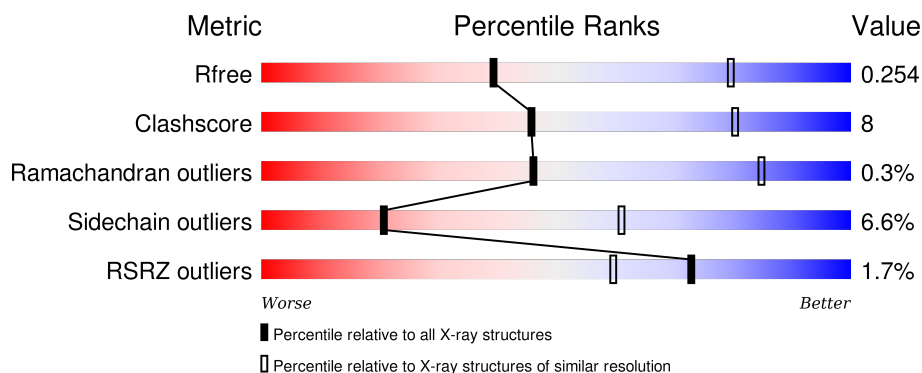
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 ≥ 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>2%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	O	234	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	B	261	<div> <div>3%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div>
2	P	261	<div> <div>5%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
3	C	248	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	199	
14	b	199	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49084 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	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	6			
1	O	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	5			
3	Q	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	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
			1777	1116	294	356	11			
4	R	233	Total	C	N	O	S	0	0	0
			1777	1116	294	356	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			

- 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			

- 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			

- Molecule 8 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			
8	V	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			

- 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
			1591	1013	265	294	19			
9	W	204	Total	C	N	O	S	0	0	0
			1591	1013	265	294	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

- Molecule 11 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			
11	Y	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			

- 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
			1653	1047	284	312	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1653	1047	284	312	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			

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			
14	b	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			

- Molecule 15 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	I	0	0
			1	1		
15	E	1	Total	I	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total I 1 1	0	0
15	b	2	Total I 2 2	0	0
15	I	1	Total I 1 1	0	0
15	C	1	Total I 1 1	0	0
15	V	1	Total I 1 1	0	0
15	W	1	Total I 1 1	0	0
15	A	1	Total I 1 1	0	0
15	N	2	Total I 2 2	0	0
15	O	1	Total I 1 1	0	0
15	Y	1	Total I 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	P	1	Total Cl 1 1	0	0
16	G	1	Total Cl 1 1	0	0
16	Q	2	Total Cl 2 2	0	0
16	D	1	Total Cl 1 1	0	0
16	K	1	Total Cl 1 1	0	0
16	a	2	Total Cl 2 2	0	0
16	E	1	Total Cl 1 1	0	0
16	H	1	Total Cl 1 1	0	0
16	B	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	b	1	Total Cl 1 1	0	0
16	V	2	Total Cl 2 2	0	0
16	Z	1	Total Cl 1 1	0	0
16	A	1	Total Cl 1 1	0	0
16	N	2	Total Cl 2 2	0	0
16	U	1	Total Cl 1 1	0	0
16	R	1	Total Cl 1 1	0	0
16	L	1	Total Cl 1 1	0	0
16	S	1	Total Cl 1 1	0	0
16	M	1	Total Cl 1 1	0	0

- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total K 1 1	0	0
17	K	1	Total K 1 1	0	0
17	E	1	Total K 1 1	0	0
17	H	1	Total K 1 1	0	0
17	b	1	Total K 1 1	0	0
17	C	1	Total K 1 1	0	0
17	T	1	Total K 1 1	0	0
17	Y	1	Total K 1 1	0	0
17	S	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	F	1	Total	K	0	0
			1	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	20	Total	O	0	0
			20	20		
18	B	18	Total	O	0	0
			18	18		
18	C	24	Total	O	0	0
			24	24		
18	D	16	Total	O	0	0
			16	16		
18	E	22	Total	O	0	0
			22	22		
18	F	17	Total	O	0	0
			17	17		
18	G	23	Total	O	0	0
			23	23		
18	H	18	Total	O	0	0
			18	18		
18	I	18	Total	O	0	0
			18	18		
18	J	14	Total	O	0	0
			14	14		
18	K	14	Total	O	0	0
			14	14		
18	L	22	Total	O	0	0
			22	22		
18	M	24	Total	O	0	0
			24	24		
18	N	18	Total	O	0	0
			18	18		
18	O	10	Total	O	0	0
			10	10		
18	P	20	Total	O	0	0
			20	20		
18	Q	21	Total	O	0	0
			21	21		
18	R	17	Total	O	0	0
			17	17		

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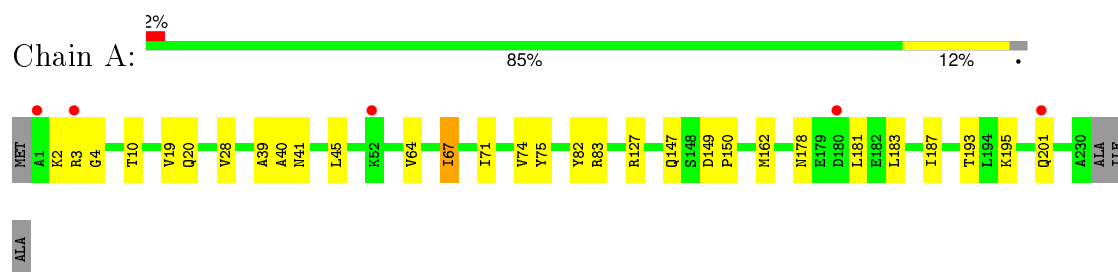
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	S	23	Total 23	O 23	0	0
18	T	24	Total 24	O 24	0	0
18	U	15	Total 15	O 15	0	0
18	V	14	Total 14	O 14	0	0
18	W	17	Total 17	O 17	0	0
18	X	15	Total 15	O 15	0	0
18	Y	26	Total 26	O 26	0	0
18	Z	25	Total 25	O 25	0	0
18	a	21	Total 21	O 21	0	0
18	b	19	Total 19	O 19	0	0

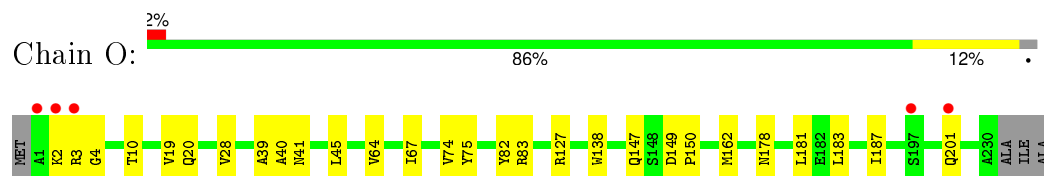
3 Residue-property plots [i](#)

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.

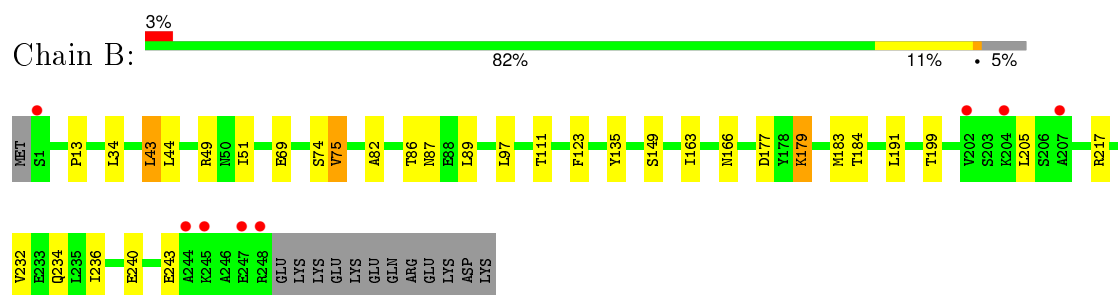
- Molecule 1: Proteasome subunit alpha type-2



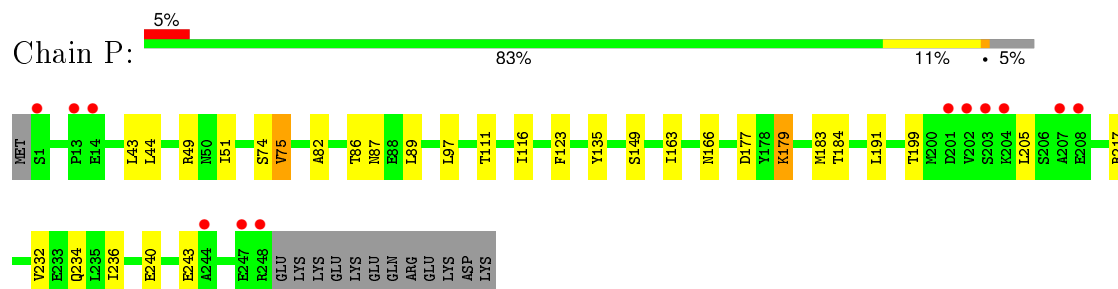
- Molecule 1: Proteasome subunit alpha type-2



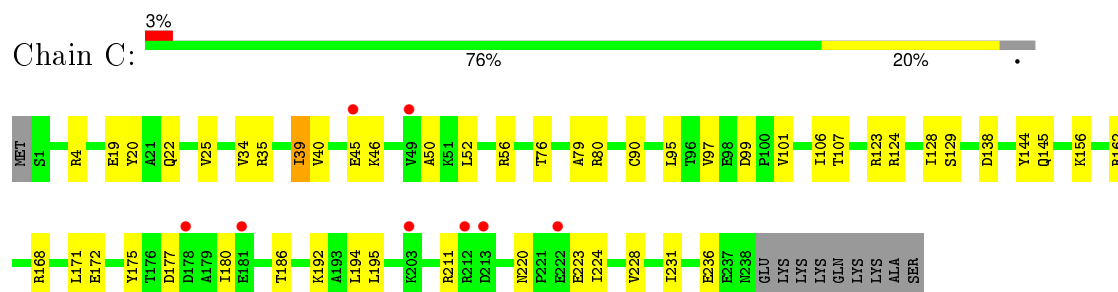
- Molecule 2: Proteasome subunit alpha type-4



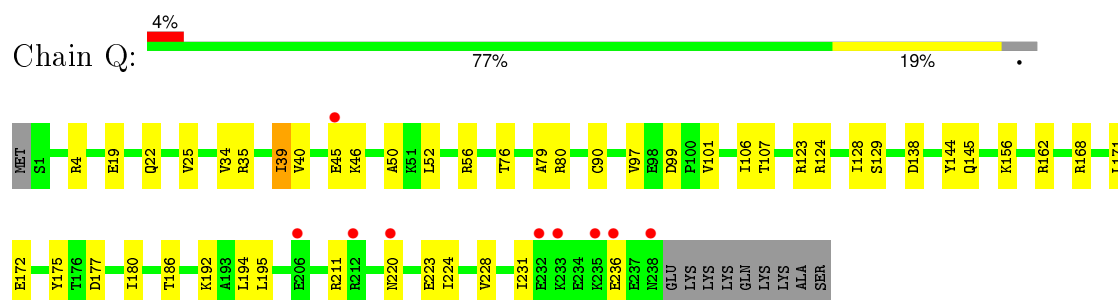
- Molecule 2: Proteasome subunit alpha type-4



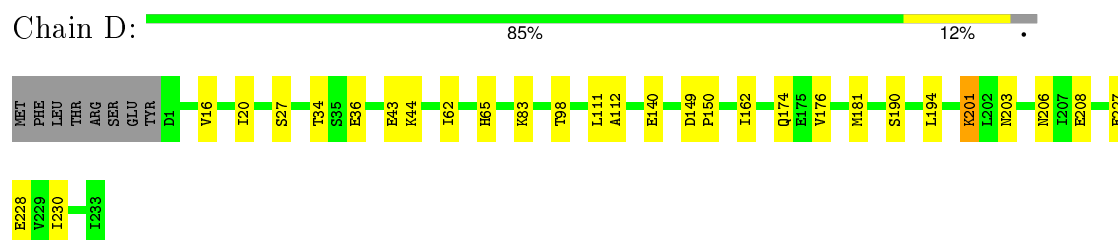
- Molecule 3: Proteasome subunit alpha type-7



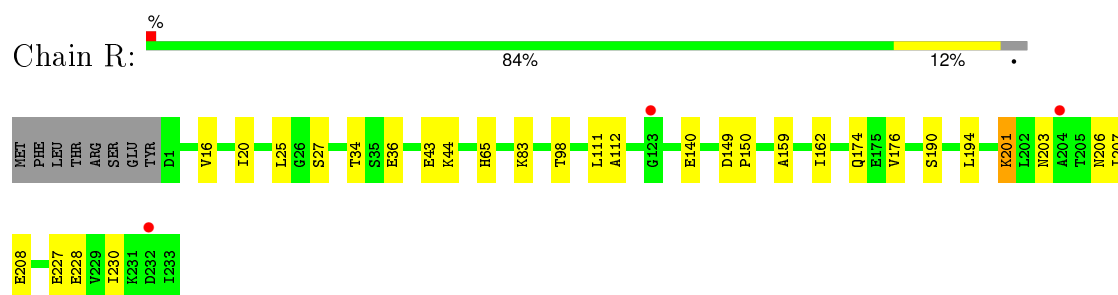
- Molecule 3: Proteasome subunit alpha type-7



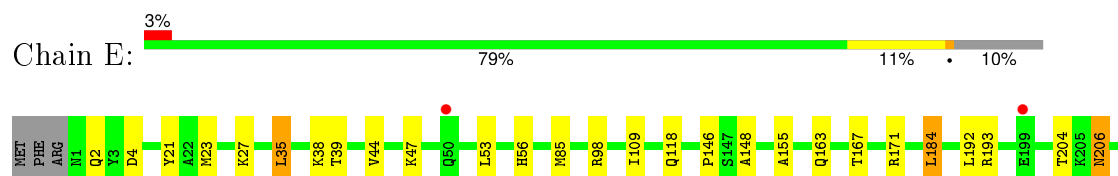
- Molecule 4: Proteasome subunit alpha type-5

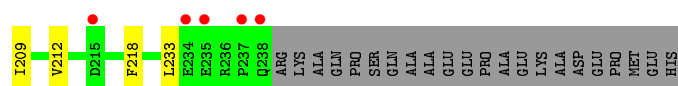


- Molecule 4: Proteasome subunit alpha type-5

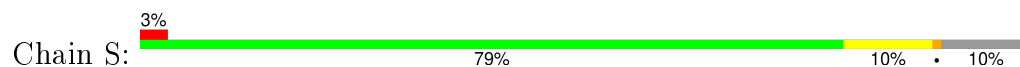


- Molecule 5: Proteasome subunit alpha type-1

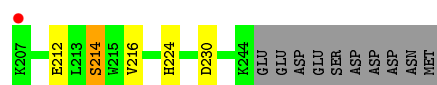
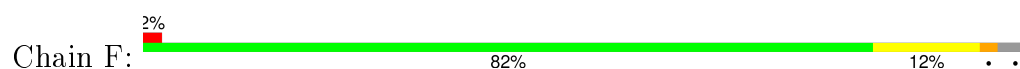




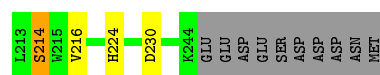
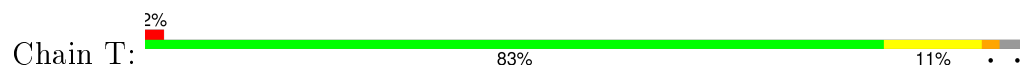
- Molecule 5: Proteasome subunit alpha type-1



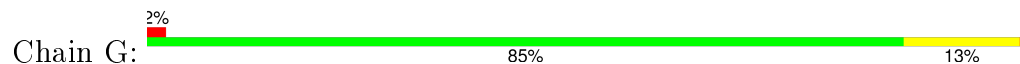
- Molecule 6: Proteasome subunit alpha type-3



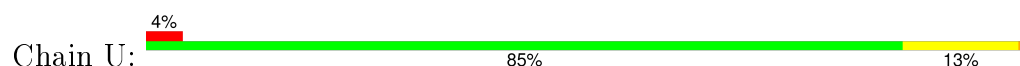
- Molecule 6: Proteasome subunit alpha type-3

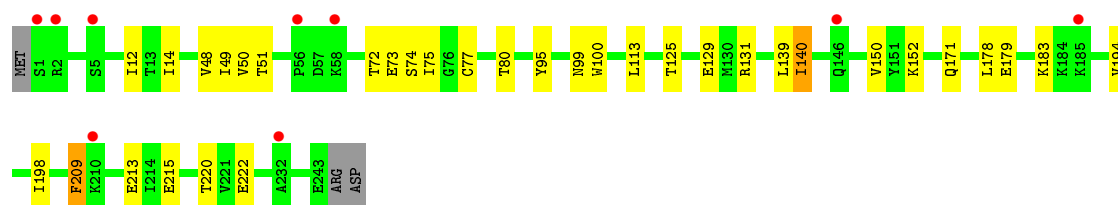


- Molecule 7: Proteasome subunit alpha type-6

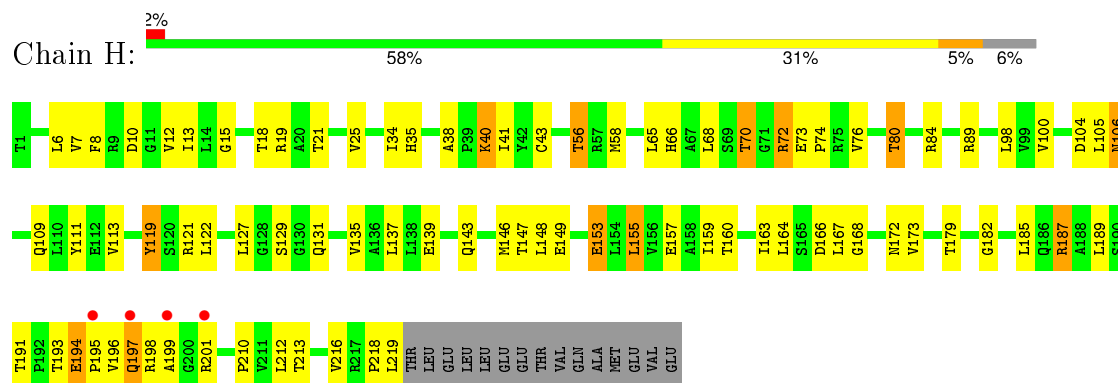


- Molecule 7: Proteasome subunit alpha type-6

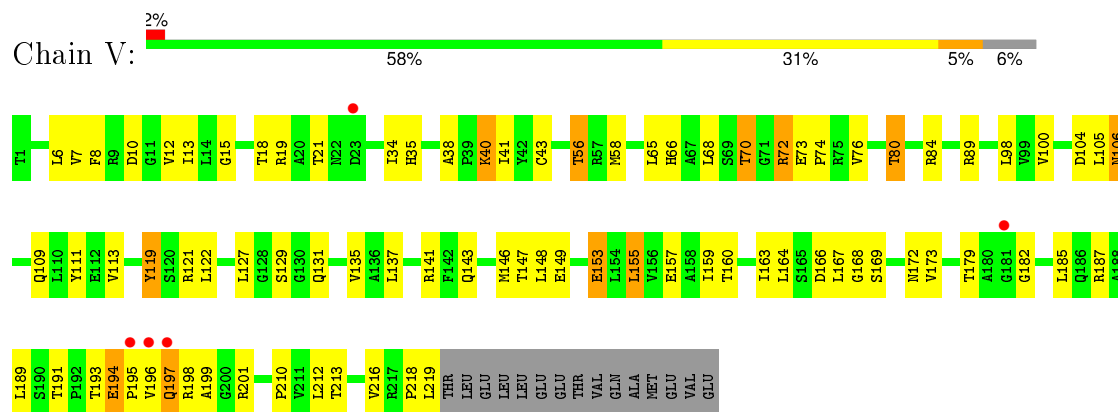




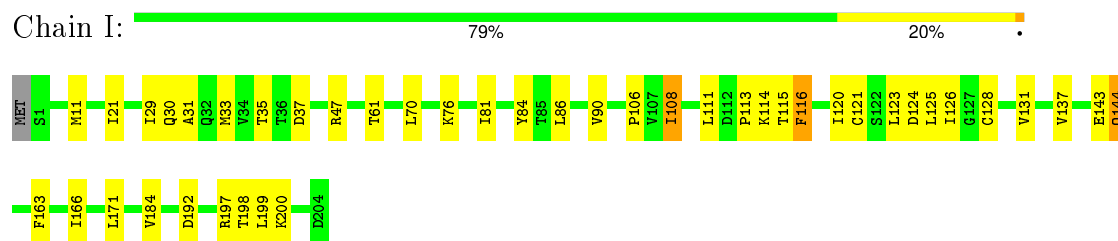
• Molecule 8: Proteasome subunit beta type-10



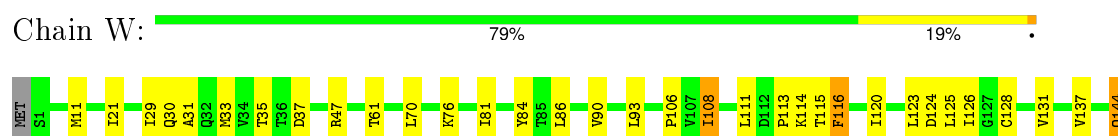
• Molecule 8: Proteasome subunit beta type-10

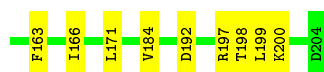


• Molecule 9: Proteasome subunit beta type-3



• Molecule 9: Proteasome subunit beta type-3





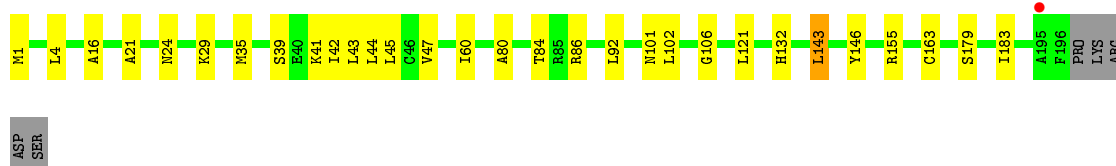
• Molecule 10: Proteasome subunit beta type-2

Chain J: 84% 13% .



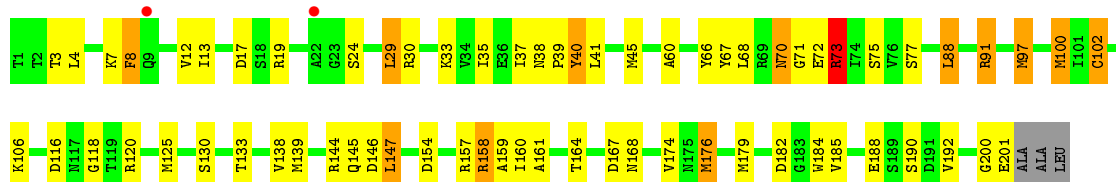
• Molecule 10: Proteasome subunit beta type-2

Chain X: 83% 14% .



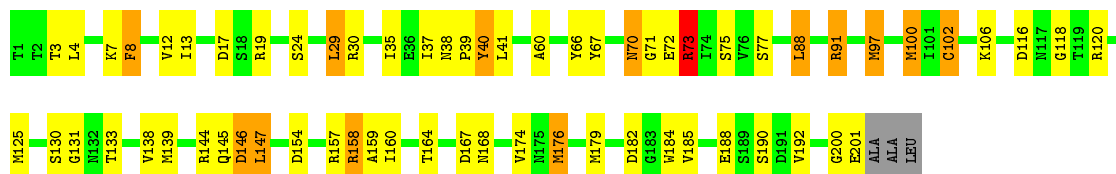
• Molecule 11: Proteasome subunit beta type-8

Chain K: 66% 26% 6% .



• Molecule 11: Proteasome subunit beta type-8

Chain Y: 67% 25% 6% .



• Molecule 12: Proteasome subunit beta type-1

Chain L: 88% 10% .



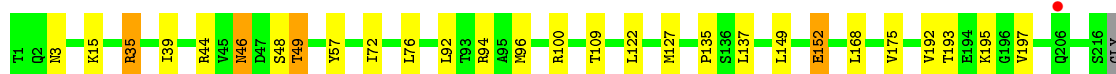
• Molecule 12: Proteasome subunit beta type-1

Chain Z: 88% 11% .



- Molecule 13: Proteasome subunit beta type-4

Chain M: 86% 11% ..



PHE
GLU

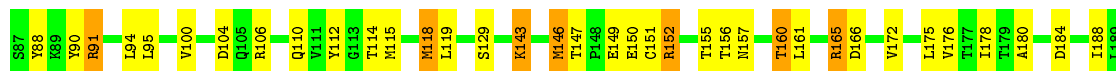
- Molecule 13: Proteasome subunit beta type-4

Chain a: 93% 5% .



- Molecule 14: Proteasome subunit beta type-9

Chain N: 59% 35% 6%



G190, D191, E192, L193, P194, E199

- Molecule 14: Proteasome subunit beta type-9

Chain b: 89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.28Å 205.22Å 161.94Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 29.83 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-3.20) 99.3 (29.83-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.239 , 0.254 0.239 , 0.254	Depositor DCC
R_{free} test set	6015 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 121329 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	49084	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, IOD, CL

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	0/1840	0.47	0/2491
1	O	0.38	1/1840 (0.1%)	0.47	0/2491
2	B	0.37	0/1980	0.48	0/2667
2	P	0.37	0/1980	0.48	0/2667
3	C	0.33	0/1903	0.48	0/2569
3	Q	0.33	0/1903	0.48	0/2569
4	D	0.36	0/1804	0.45	0/2437
4	R	0.35	0/1804	0.45	0/2437
5	E	0.37	0/1907	0.48	0/2578
5	S	0.37	0/1907	0.48	0/2578
6	F	0.38	0/1938	0.46	0/2608
6	T	0.38	0/1938	0.46	0/2608
7	G	0.37	1/1924 (0.1%)	0.46	0/2600
7	U	0.37	1/1924 (0.1%)	0.46	0/2600
8	H	0.32	0/1645	0.53	0/2235
8	V	0.32	0/1645	0.53	0/2235
9	I	0.34	0/1620	0.48	0/2185
9	W	0.34	0/1620	0.48	0/2185
10	J	0.33	0/1602	0.47	0/2167
10	X	0.32	0/1602	0.47	0/2167
11	K	0.40	0/1597	0.51	0/2151
11	Y	0.40	0/1597	0.50	0/2151
12	L	0.32	0/1684	0.46	0/2271
12	Z	0.32	0/1684	0.46	0/2271
13	M	0.40	0/1718	0.48	0/2325
13	a	0.40	1/1718 (0.1%)	0.48	0/2325
14	N	0.35	0/1526	0.50	0/2071
14	b	0.35	0/1526	0.50	0/2071
All	All	0.36	4/49376 (0.0%)	0.48	0/66710

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	138	TRP	CD2-CE2	5.08	1.47	1.41
13	a	209	TRP	CD2-CE2	5.06	1.47	1.41
7	G	188	TRP	CD2-CE2	5.05	1.47	1.41
7	U	100	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 ⓘ

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	1801	0	1800	15	0
1	O	1801	0	1800	14	0
2	B	1950	0	1973	18	0
2	P	1950	0	1973	12	0
3	C	1876	0	1902	22	0
3	Q	1876	0	1902	20	0
4	D	1777	0	1767	15	0
4	R	1777	0	1767	15	0
5	E	1872	0	1859	18	0
5	S	1872	0	1858	18	0
6	F	1903	0	1894	20	0
6	T	1903	0	1894	17	0
7	G	1890	0	1900	18	0
7	U	1890	0	1900	19	0
8	H	1619	0	1643	69	0
8	V	1619	0	1643	65	0
9	I	1591	0	1612	23	0
9	W	1591	0	1612	23	0
10	J	1570	0	1573	16	0
10	X	1570	0	1573	17	0
11	K	1566	0	1518	71	0
11	Y	1566	0	1518	69	0
12	L	1653	0	1652	24	0
12	Z	1653	0	1652	26	0
13	M	1685	0	1664	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	1685	0	1664	0	0
14	N	1498	0	1478	59	0
14	b	1498	0	1478	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	E	1	0	0	1	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	2	0	0	0	0
15	O	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	b	2	0	0	0	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	D	1	0	0	0	0
16	E	1	0	0	0	0
16	G	1	0	0	1	0
16	H	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	N	2	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	0	0
16	R	1	0	0	0	0
16	S	1	0	0	1	0
16	U	1	0	0	1	0
16	V	2	0	0	0	0
16	Z	1	0	0	0	0
16	a	2	0	0	0	0
16	b	1	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
17	E	1	0	0	0	0
17	F	1	0	0	0	0
17	H	1	0	0	0	0
17	K	1	0	0	0	0
17	S	1	0	0	0	0
17	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Y	1	0	0	0	0
17	b	1	0	0	0	0
18	A	20	0	0	0	0
18	B	18	0	0	2	0
18	C	24	0	0	0	0
18	D	16	0	0	0	0
18	E	22	0	0	0	0
18	F	17	0	0	0	0
18	G	23	0	0	1	0
18	H	18	0	0	1	0
18	I	18	0	0	0	0
18	J	14	0	0	0	0
18	K	14	0	0	0	0
18	L	22	0	0	0	0
18	M	24	0	0	1	0
18	N	18	0	0	0	0
18	O	10	0	0	0	0
18	P	20	0	0	0	0
18	Q	21	0	0	1	0
18	R	17	0	0	0	0
18	S	23	0	0	2	0
18	T	24	0	0	0	0
18	U	15	0	0	4	0
18	V	14	0	0	0	0
18	W	17	0	0	1	0
18	X	15	0	0	1	0
18	Y	26	0	0	1	0
18	Z	25	0	0	1	0
18	a	21	0	0	0	0
18	b	19	0	0	0	0
All	All	49084	0	48469	650	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 8.

The worst 5 of 650 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)
11:Y:125:MET:HE2	11:Y:139:MET:HE3	1.21	1.18
11:K:125:MET:HE2	11:K:139:MET:HE3	1.23	1.16
11:K:144:ARG:O	11:K:147:LEU:HD12	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:144:ARG:O	11:Y:147:LEU:HD12	1.57	1.04
14:N:152:ARG:HH21	14:N:152:ARG:HG3	1.26	1.00

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	228/234 (97%)	219 (96%)	8 (4%)	1 (0%)	39	80
1	O	228/234 (97%)	220 (96%)	7 (3%)	1 (0%)	39	80
2	B	246/261 (94%)	241 (98%)	5 (2%)	0	100	100
2	P	246/261 (94%)	241 (98%)	5 (2%)	0	100	100
3	C	236/248 (95%)	227 (96%)	9 (4%)	0	100	100
3	Q	236/248 (95%)	227 (96%)	9 (4%)	0	100	100
4	D	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	39	80
4	R	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	39	80
5	E	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
5	S	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
6	F	242/255 (95%)	236 (98%)	5 (2%)	1 (0%)	39	80
6	T	242/255 (95%)	236 (98%)	5 (2%)	1 (0%)	39	80
7	G	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	U	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
8	H	217/234 (93%)	213 (98%)	3 (1%)	1 (0%)	34	78
8	V	217/234 (93%)	213 (98%)	3 (1%)	1 (0%)	34	78
9	I	202/205 (98%)	192 (95%)	8 (4%)	2 (1%)	19	65
9	W	202/205 (98%)	192 (95%)	8 (4%)	2 (1%)	19	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	194/201 (96%)	188 (97%)	5 (3%)	1 (0%)	34	78
10	X	194/201 (96%)	188 (97%)	5 (3%)	1 (0%)	34	78
11	K	199/204 (98%)	194 (98%)	4 (2%)	1 (0%)	34	78
11	Y	199/204 (98%)	194 (98%)	4 (2%)	1 (0%)	34	78
12	L	211/213 (99%)	206 (98%)	4 (2%)	1 (0%)	34	78
12	Z	211/213 (99%)	206 (98%)	4 (2%)	1 (0%)	34	78
13	M	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
13	a	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
14	N	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
14	b	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
All	All	6188/6446 (96%)	5999 (97%)	171 (3%)	18 (0%)	46	85

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	216	VAL
8	H	195	PRO
9	I	30	GLN
10	J	24	ASN
6	T	216	VAL

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%)	182 (96%)	7 (4%)	41	79
1	O	189/191 (99%)	182 (96%)	7 (4%)	41	79
2	B	208/221 (94%)	194 (93%)	14 (7%)	20	60
2	P	208/221 (94%)	193 (93%)	15 (7%)	18	57
3	C	202/211 (96%)	188 (93%)	14 (7%)	19	59
3	Q	202/211 (96%)	188 (93%)	14 (7%)	19	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	195/203 (96%)	191 (98%)	4 (2%)	61	88
4	R	195/203 (96%)	190 (97%)	5 (3%)	54	85
5	E	204/224 (91%)	198 (97%)	6 (3%)	50	83
5	S	204/224 (91%)	198 (97%)	6 (3%)	50	83
6	F	200/211 (95%)	192 (96%)	8 (4%)	38	77
6	T	200/211 (95%)	192 (96%)	8 (4%)	38	77
7	G	207/210 (99%)	200 (97%)	7 (3%)	44	80
7	U	207/210 (99%)	200 (97%)	7 (3%)	44	80
8	H	169/183 (92%)	133 (79%)	36 (21%)	1	7
8	V	169/183 (92%)	133 (79%)	36 (21%)	1	7
9	I	174/175 (99%)	162 (93%)	12 (7%)	19	59
9	W	174/175 (99%)	162 (93%)	12 (7%)	19	59
10	J	166/171 (97%)	164 (99%)	2 (1%)	78	93
10	X	166/171 (97%)	164 (99%)	2 (1%)	78	93
11	K	165/166 (99%)	142 (86%)	23 (14%)	4	20
11	Y	165/166 (99%)	142 (86%)	23 (14%)	4	20
12	L	178/178 (100%)	173 (97%)	5 (3%)	51	84
12	Z	178/178 (100%)	173 (97%)	5 (3%)	51	84
13	M	178/180 (99%)	167 (94%)	11 (6%)	23	64
13	a	178/180 (99%)	167 (94%)	11 (6%)	23	64
14	N	155/155 (100%)	134 (86%)	21 (14%)	5	22
14	b	155/155 (100%)	134 (86%)	21 (14%)	5	22
All	All	5180/5358 (97%)	4838 (93%)	342 (7%)	21	61

5 of 342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	77	LEU
2	P	243	GLU
13	a	94	ARG
14	N	104	ASP
1	O	28	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	38	HIS
2	P	122	GLN
13	a	104	ASN
14	N	81	ASN
1	O	111	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](#)

Of 47 ligands modelled in this entry, 47 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	230/234 (98%)	0.00	5 (2%) 65 50	58, 92, 140, 157	0
1	O	230/234 (98%)	0.00	5 (2%) 65 50	59, 90, 134, 147	0
2	B	248/261 (95%)	-0.07	8 (3%) 51 36	55, 86, 155, 209	0
2	P	248/261 (95%)	0.00	12 (4%) 34 21	56, 88, 149, 188	0
3	C	238/248 (95%)	0.07	8 (3%) 49 34	50, 89, 165, 230	0
3	Q	238/248 (95%)	0.16	9 (3%) 44 29	54, 99, 172, 252	0
4	D	233/241 (96%)	-0.09	0 100 100	49, 83, 136, 175	0
4	R	233/241 (96%)	-0.01	3 (1%) 79 67	59, 95, 151, 191	0
5	E	238/263 (90%)	-0.00	7 (2%) 55 41	53, 85, 135, 172	0
5	S	238/263 (90%)	-0.03	7 (2%) 55 41	49, 80, 136, 160	0
6	F	244/255 (95%)	0.01	5 (2%) 68 54	54, 91, 138, 160	0
6	T	244/255 (95%)	-0.02	6 (2%) 61 47	49, 81, 125, 141	0
7	G	243/246 (98%)	0.06	5 (2%) 67 52	62, 98, 157, 198	0
7	U	243/246 (98%)	0.01	9 (3%) 45 30	59, 88, 137, 166	0
8	H	219/234 (93%)	-0.24	4 (1%) 71 58	39, 72, 123, 151	0
8	V	219/234 (93%)	-0.22	5 (2%) 64 49	36, 70, 116, 147	0
9	I	204/205 (99%)	-0.33	0 100 100	42, 61, 103, 127	0
9	W	204/205 (99%)	-0.30	0 100 100	46, 65, 107, 132	0
10	J	196/201 (97%)	-0.35	1 (0%) 91 87	45, 62, 89, 113	0
10	X	196/201 (97%)	-0.28	1 (0%) 91 87	47, 65, 98, 118	0
11	K	201/204 (98%)	-0.38	2 (0%) 84 75	34, 59, 92, 104	0
11	Y	201/204 (98%)	-0.31	0 100 100	39, 65, 99, 111	0
12	L	213/213 (100%)	-0.27	0 100 100	43, 61, 90, 118	0
12	Z	213/213 (100%)	-0.34	1 (0%) 91 87	44, 57, 88, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.39	1 (0%) 91 87	42, 61, 94, 108	0
13	a	216/219 (98%)	-0.40	0 100 100	41, 57, 87, 117	0
14	N	199/199 (100%)	-0.40	0 100 100	35, 63, 92, 102	0
14	b	199/199 (100%)	-0.36	0 100 100	37, 64, 92, 101	0
All	All	6244/6446 (96%)	-0.15	104 (1%) 73 60	34, 75, 138, 252	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	1	SER	7.4
6	F	1	SER	7.2
5	E	238	GLN	6.7
7	U	1	SER	6.7
6	F	2	SER	6.5

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, 95th 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 ²)	Q<0.9
16	CL	S	262	1/1	0.98	0.23	0.73	30,30,30,30	0
16	CL	N	202	1/1	0.94	0.20	0.69	24,24,24,24	0
17	K	H	236	1/1	0.92	0.19	0.35	30,30,30,30	0
16	CL	V	236	1/1	0.98	0.20	0.16	27,27,27,27	0
16	CL	R	234	1/1	0.87	0.18	0.04	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	CL	G	246	1/1	0.83	0.18	-0.11	28,28,28,28	0
16	CL	A	235	1/1	0.96	0.22	-0.58	23,23,23,23	0
16	CL	b	203	1/1	0.93	0.15	-0.78	23,23,23,23	0
16	CL	Q	248	1/1	0.97	0.22	-0.94	34,34,34,34	0
16	CL	N	203	1/1	0.94	0.17	-1.11	33,33,33,33	0
16	CL	H	237	1/1	0.99	0.13	-1.21	29,29,29,29	0
16	CL	K	207	1/1	0.97	0.08	-1.47	27,27,27,27	0
17	K	T	255	1/1	0.82	0.10	-1.71	40,40,40,40	0
17	K	Y	206	1/1	0.95	0.10	-1.81	29,29,29,29	0
16	CL	E	263	1/1	0.99	0.10	-1.82	42,42,42,42	0
17	K	D	234	1/1	0.92	0.11	-2.02	42,42,42,42	0
17	K	b	202	1/1	0.95	0.12	-2.10	30,30,30,30	0
17	K	E	262	1/1	0.90	0.08	-2.12	46,46,46,46	0
16	CL	V	237	1/1	1.00	0.13	-2.29	20,20,20,20	0
16	CL	U	246	1/1	0.72	0.15	-2.34	30,30,30,30	0
16	CL	D	235	1/1	0.98	0.12	-2.43	41,41,41,41	0
15	IOD	E	261	1/1	0.99	0.07	-2.50	92,92,92,92	0
16	CL	Q	249	1/1	0.97	0.20	-	35,35,35,35	0
17	K	C	249	1/1	0.95	0.12	-	36,36,36,36	0
16	CL	M	220	1/1	0.96	0.16	-	31,31,31,31	0
16	CL	a	221	1/1	0.99	0.06	-	20,20,20,20	0
17	K	F	255	1/1	0.90	0.09	-	48,48,48,48	0
15	IOD	N	201	1/1	0.99	0.24	-	168,168,168,168	0
15	IOD	b	201	1/1	0.99	0.09	-	82,82,82,82	0
15	IOD	I	205	1/1	0.99	0.06	-	79,79,79,79	0
16	CL	Z	214	1/1	0.97	0.06	-	24,24,24,24	0
15	IOD	V	235	1/1	0.99	0.03	-	68,68,68,68	0
15	IOD	O	234	1/1	0.99	0.06	-	83,83,83,83	0
15	IOD	C	248	1/1	0.99	0.07	-	86,86,86,86	0
17	K	K	206	1/1	0.94	0.12	-	43,43,43,43	0
16	CL	P	261	1/1	0.94	0.07	-	27,27,27,27	0
15	IOD	H	235	1/1	0.99	0.03	-	59,59,59,59	0
16	CL	a	220	1/1	0.96	0.19	-	41,41,41,41	0
16	CL	L	214	1/1	0.98	0.13	-	28,28,28,28	0
15	IOD	Y	205	1/1	1.00	0.07	-	69,69,69,69	0
15	IOD	b	200	1/1	0.99	0.10	-	30,30,30,30	0
16	CL	B	261	1/1	0.96	0.09	-	34,34,34,34	0
15	IOD	A	234	1/1	0.99	0.11	-	76,76,76,76	0
15	IOD	K	205	1/1	1.00	0.02	-	64,64,64,64	0
15	IOD	W	205	1/1	0.99	0.09	-	83,83,83,83	0
15	IOD	N	200	1/1	0.99	0.03	-	49,49,49,49	0
17	K	S	261	1/1	0.91	0.12	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.