



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:41 pm BST

PDB ID : 6HWC  
Title : Yeast 20S proteasome beta2-G45A mutant  
Authors : Huber, E.M.; Groll, M.  
Deposited on : 2018-10-11  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

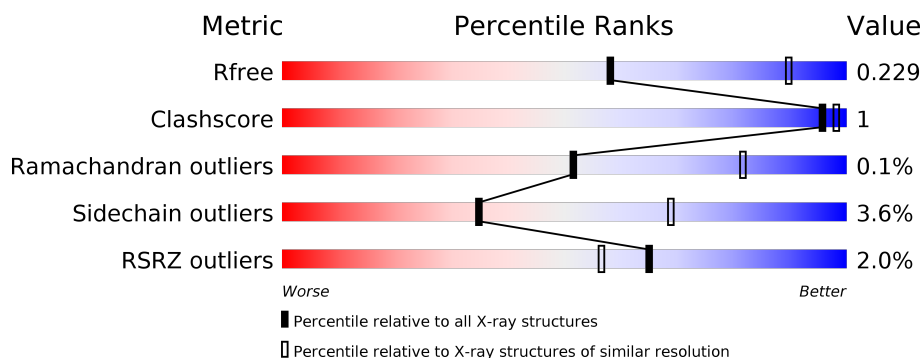
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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  $\leq 5\%$ . 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	250	<div> <div>3%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>2%</div> <div>98%</div> <div>•</div> </div>
2	B	258	<div> <div>4%</div> <div>87%</div> <div>5% • 5%</div> </div>
2	P	258	<div> <div>3%</div> <div>88%</div> <div>6% • 5%</div> </div>
3	C	254	<div> <div>4%</div> <div>87%</div> <div>7% • 6%</div> </div>
3	Q	254	<div> <div>7%</div> <div>87%</div> <div>7% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50117 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1720	1083	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1720	1083	298	332	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	45	ALA	GLY	engineered mutation	UNP P25043
V	45	ALA	GLY	engineered mutation	UNP P25043

- 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
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

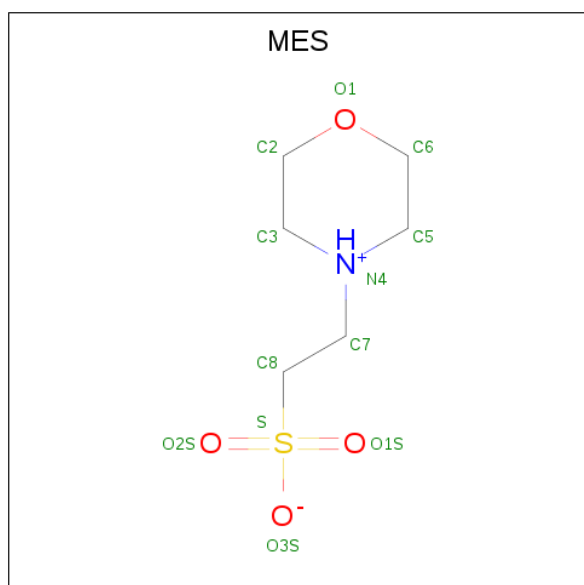
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0

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

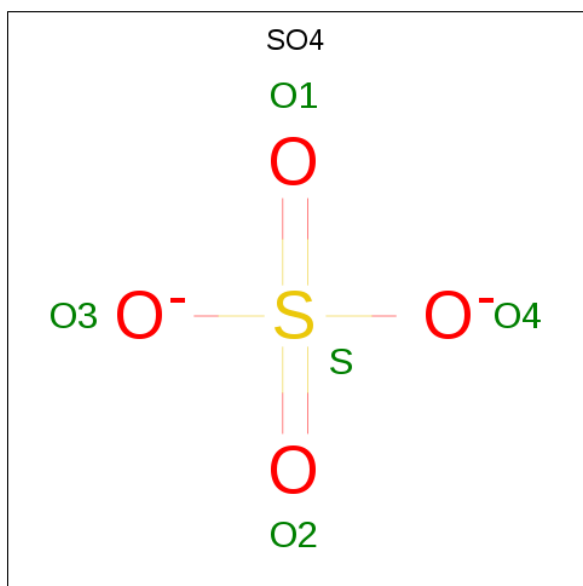
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	V	1	Total	O	S	0	0
			5	4	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	23	Total	O	0	0
			23	23		
19	B	22	Total	O	0	0
			22	22		
19	C	23	Total	O	0	0
			23	23		
19	D	27	Total	O	0	0
			27	27		
19	E	17	Total	O	0	0
			17	17		
19	F	21	Total	O	0	0
			21	21		
19	G	31	Total	O	0	0
			31	31		
19	H	37	Total	O	0	0
			37	37		

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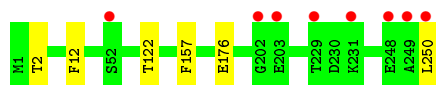
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	I	21	Total O 21 21	0	0
19	J	20	Total O 20 20	0	0
19	K	39	Total O 39 39	0	0
19	L	35	Total O 35 35	0	0
19	M	32	Total O 32 32	0	0
19	N	29	Total O 29 29	0	0
19	O	10	Total O 10 10	0	0
19	P	21	Total O 21 21	0	0
19	Q	18	Total O 18 18	0	0
19	R	27	Total O 27 27	0	0
19	S	22	Total O 22 22	0	0
19	T	20	Total O 20 20	0	0
19	U	27	Total O 27 27	0	0
19	V	26	Total O 26 26	0	0
19	W	25	Total O 25 25	0	0
19	X	17	Total O 17 17	0	0
19	Y	27	Total O 27 27	0	0
19	Z	27	Total O 27 27	0	0
19	a	40	Total O 40 40	0	0
19	b	38	Total O 38 38	0	0

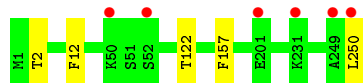
### 3 Residue-property plots [i](#)

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.

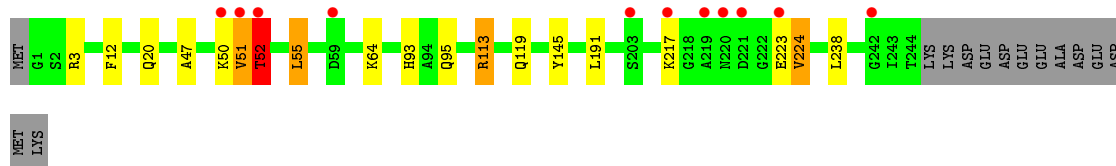
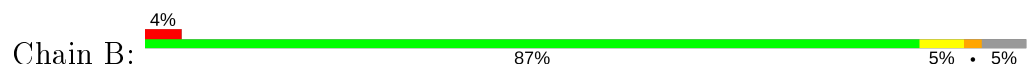
- Molecule 1: Proteasome subunit alpha type-2



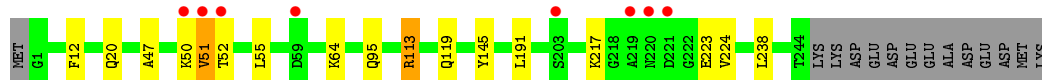
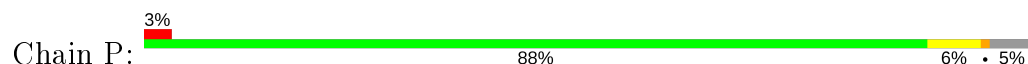
- Molecule 1: Proteasome subunit alpha type-2



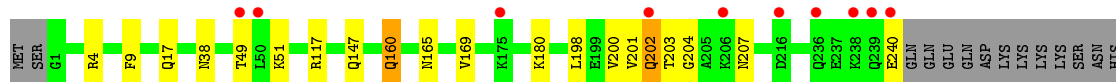
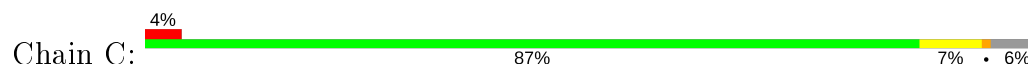
- Molecule 2: Proteasome subunit alpha type-3



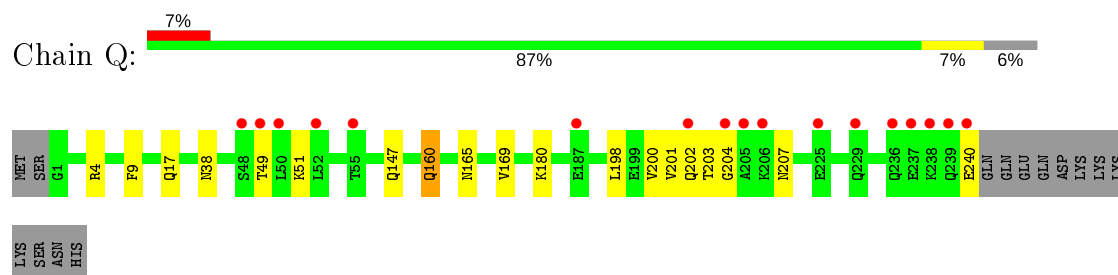
- Molecule 2: Proteasome subunit alpha type-3



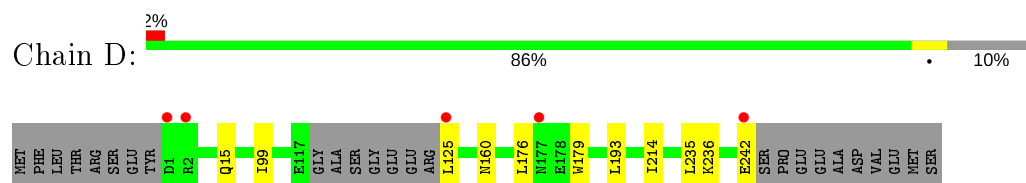
- Molecule 3: Proteasome subunit alpha type-4



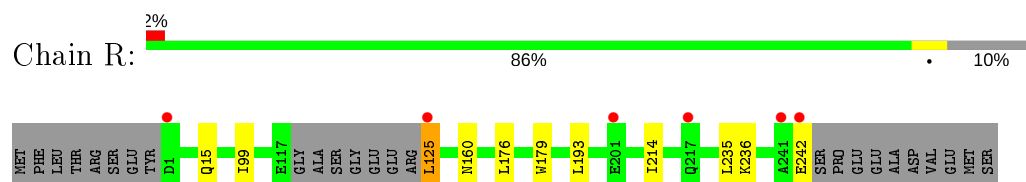
- Molecule 3: Proteasome subunit alpha type-4



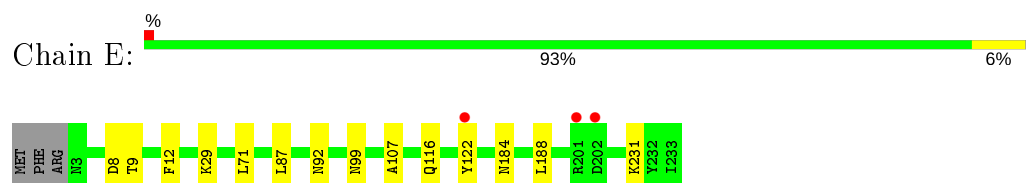
- Molecule 4: Proteasome subunit alpha type-5



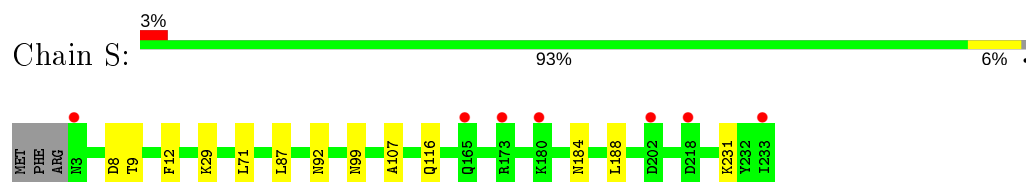
- Molecule 4: Proteasome subunit alpha type-5



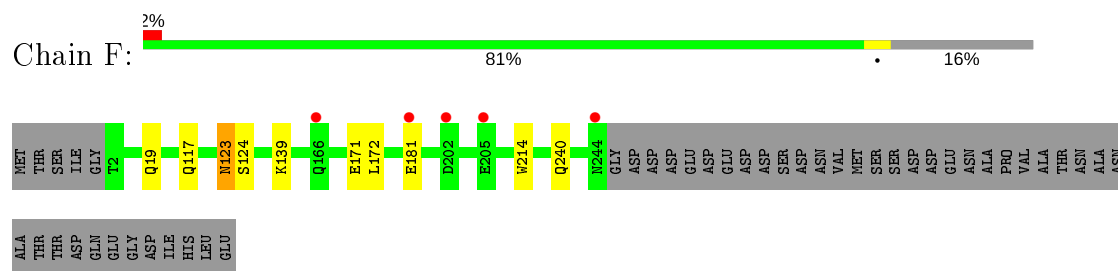
- Molecule 5: Proteasome subunit alpha type-6



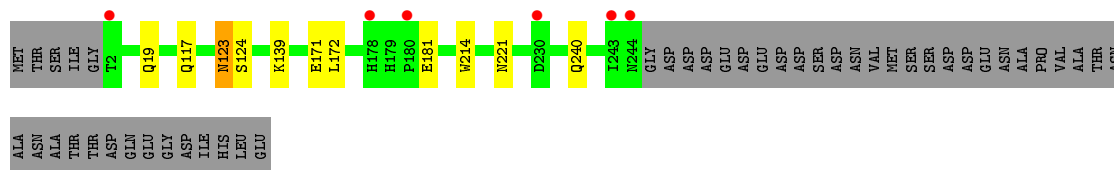
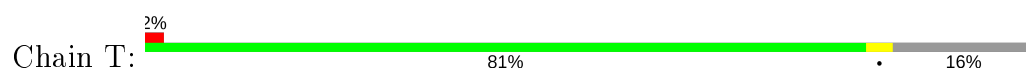
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7



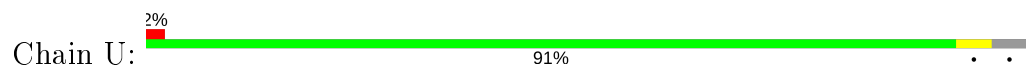
- Molecule 6: Probable proteasome subunit alpha type-7



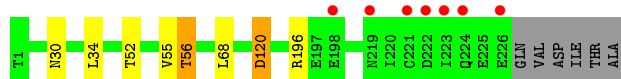
- Molecule 7: Proteasome subunit alpha type-1



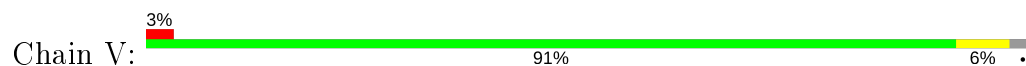
- Molecule 7: Proteasome subunit alpha type-1



- Molecule 8: Proteasome subunit beta type-2



- Molecule 8: Proteasome subunit beta type-2

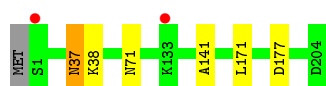


- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3





- Molecule 10: Proteasome subunit beta type-4



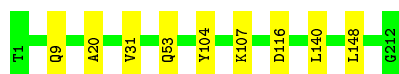
- Molecule 10: Proteasome subunit beta type-4



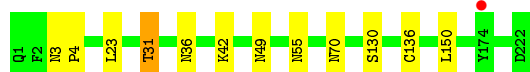
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



- Molecule 12: Proteasome subunit beta type-6

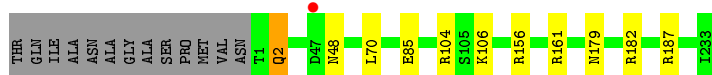


- Molecule 12: Proteasome subunit beta type-6

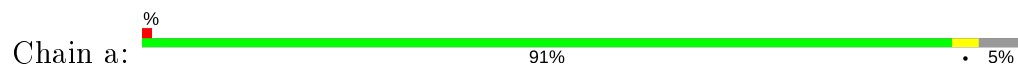


- Molecule 13: Proteasome subunit beta type-7

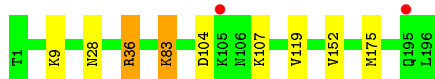




- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.42Å 301.17Å 144.61Å 90.00° 113.03° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.80) 96.2 (15.00-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.195 , 0.224 0.203 , 0.229	Depositor DCC
$R_{free}$ test set	12455 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50117	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, MES, 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	0.37	0/1952	0.57	0/2642
1	O	0.37	0/1952	0.57	0/2642
2	B	0.46	1/1934 (0.1%)	0.73	3/2618 (0.1%)
2	P	0.48	1/1934 (0.1%)	0.73	3/2618 (0.1%)
3	C	0.39	0/1910	0.64	1/2586 (0.0%)
3	Q	0.38	0/1910	0.64	0/2586
4	D	0.36	0/1837	0.59	0/2475
4	R	0.36	0/1837	0.59	0/2475
5	E	0.37	0/1800	0.58	0/2433
5	S	0.36	0/1800	0.59	0/2433
6	F	0.37	0/1932	0.56	0/2609
6	T	0.36	0/1932	0.56	0/2609
7	G	0.38	0/1945	0.58	0/2634
7	U	0.37	0/1945	0.58	0/2634
8	H	0.35	0/1751	0.59	0/2375
8	V	0.34	0/1751	0.59	0/2375
9	I	0.37	0/1611	0.59	0/2174
9	W	0.37	0/1611	0.60	0/2174
10	J	0.37	0/1589	0.61	0/2142
10	X	0.37	0/1589	0.61	0/2142
11	K	0.36	0/1681	0.60	0/2274
11	Y	0.34	0/1681	0.59	0/2274
12	L	0.37	0/1795	0.60	0/2420
12	Z	0.37	0/1795	0.59	0/2420
13	M	0.38	0/1855	0.65	0/2514
13	a	0.38	0/1855	0.65	0/2514
14	N	0.35	0/1541	0.58	0/2087
14	b	0.35	0/1541	0.58	0/2087
All	All	0.38	2/50266 (0.0%)	0.61	7/67966 (0.0%)

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	51	VAL	CB-CG2	-9.58	1.32	1.52
2	B	51	VAL	CB-CG1	-7.84	1.36	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	VAL	CA-CB-CG1	-9.99	95.92	110.90
2	P	51	VAL	CB-CA-C	-9.48	93.40	111.40
2	P	51	VAL	CA-CB-CG2	-9.25	97.03	110.90
2	P	224	VAL	CG1-CB-CG2	6.03	120.54	110.90
2	B	224	VAL	CG1-CB-CG2	5.74	120.08	110.90
2	B	51	VAL	CB-CA-C	-5.59	100.78	111.40
3	C	202	GLN	CB-CG-CD	5.13	124.95	111.60

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	1915	0	1929	2	0
1	O	1915	0	1929	1	0
2	B	1904	0	1904	16	0
2	P	1904	0	1904	11	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	2	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	6	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	2	0
7	U	1907	0	1901	1	0
8	H	1720	0	1721	2	0
8	V	1720	0	1721	6	0
9	I	1581	0	1574	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	1581	0	1574	5	0
10	J	1561	0	1569	1	0
10	X	1561	0	1569	1	0
11	K	1644	0	1595	4	0
11	Y	1644	0	1595	1	0
12	L	1757	0	1711	7	0
12	Z	1757	0	1711	8	0
13	M	1824	0	1832	4	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	4	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	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	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	12	0	13	0	0
18	V	5	0	0	0	0
19	A	23	0	0	0	0
19	B	22	0	0	2	0
19	C	23	0	0	1	0
19	D	27	0	0	0	0
19	E	17	0	0	0	0
19	F	21	0	0	0	0
19	G	31	0	0	0	0
19	H	37	0	0	0	0
19	I	21	0	0	0	0
19	J	20	0	0	0	0
19	K	39	0	0	1	0
19	L	35	0	0	0	0
19	M	32	0	0	2	0
19	N	29	0	0	1	0
19	O	10	0	0	0	0
19	P	21	0	0	1	0
19	Q	18	0	0	0	0
19	R	27	0	0	1	0
19	S	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	T	20	0	0	0	0
19	U	27	0	0	0	0
19	V	26	0	0	0	0
19	W	25	0	0	0	0
19	X	17	0	0	0	0
19	Y	27	0	0	0	0
19	Z	27	0	0	0	0
19	a	40	0	0	0	0
19	b	38	0	0	0	0
All	All	50117	0	49147	100	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 1.

All (100) 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)
3:C:202:GLN:O	3:C:202:GLN:HG2	1.74	0.86
2:B:51:VAL:CG2	2:B:51:VAL:O	2.25	0.83
8:V:52:THR:O	8:V:56:THR:OG1	2.04	0.76
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.36	0.72
8:H:52:THR:O	8:H:56:THR:OG1	2.08	0.71
2:B:145:TYR:OH	2:B:217:LYS:N	2.24	0.70
2:P:145:TYR:OH	2:P:217:LYS:N	2.24	0.70
8:H:120:ASP:OD1	14:N:28:ASN:ND2	2.26	0.69
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.41	0.66
2:B:51:VAL:HG22	2:B:51:VAL:O	1.96	0.66
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.61	0.65
3:Q:202:GLN:O	3:Q:202:GLN:HG3	1.96	0.65
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.63	0.63
2:B:12:PHE:H	3:C:17:GLN:HE22	1.47	0.61
6:T:123:ASN:HD22	6:T:124:SER:N	1.99	0.60
6:F:123:ASN:HD22	6:F:124:SER:N	1.99	0.59
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.67	0.59
5:S:12:PHE:H	6:T:19:GLN:HE22	1.49	0.59
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.66	0.58
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.86	0.57
7:G:23:PHE:O	7:G:26:THR:HB	2.04	0.57
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.53	0.57
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.57
3:C:117:ARG:NH1	19:C:301:HOH:O	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.88	0.56
1:O:12:PHE:H	2:P:20:GLN:HE22	1.53	0.56
5:E:12:PHE:H	6:F:19:GLN:HE22	1.53	0.56
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.55	0.55
6:F:123:ASN:C	6:F:123:ASN:HD22	2.10	0.55
13:M:2:GLN:NE2	19:M:301:HOH:O	2.38	0.55
3:Q:203:THR:HB	3:Q:207:ASN:ND2	2.22	0.55
2:B:145:TYR:HH	2:B:217:LYS:N	2.04	0.54
2:P:145:TYR:HH	2:P:217:LYS:N	2.05	0.54
3:C:203:THR:HB	3:C:207:ASN:ND2	2.22	0.53
6:T:123:ASN:HD22	6:T:123:ASN:C	2.12	0.52
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.06	0.52
2:B:51:VAL:O	2:B:51:VAL:HG23	2.07	0.52
14:N:36:ARG:NH1	19:N:301:HOH:O	2.42	0.52
2:P:113:ARG:NE	19:P:301:HOH:O	2.36	0.52
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.08	0.52
1:A:12:PHE:H	2:B:20:GLN:HE22	1.58	0.52
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.04	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.51
2:P:51:VAL:HG12	2:P:51:VAL:O	2.10	0.50
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.77	0.50
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.94	0.49
3:C:203:THR:HB	3:C:207:ASN:HD22	1.77	0.49
2:B:93:HIS:HB3	19:B:301:HOH:O	2.12	0.48
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.94	0.48
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.94	0.48
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.77	0.48
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.95	0.48
3:Q:203:THR:HB	3:Q:207:ASN:HD22	1.78	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.95	0.48
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.27	0.48
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.79	0.47
8:V:22:GLN:HG3	8:V:22:GLN:O	2.14	0.47
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.79	0.47
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.62	0.47
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.27	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.47
13:M:106:LYS:HE3	19:M:326:HOH:O	2.14	0.47
2:B:51:VAL:H	2:B:51:VAL:HG12	1.47	0.46
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:37:ASN:HD22	9:I:37:ASN:C	2.19	0.46
14:N:152:VAL:HA	14:N:175:MET:HE1	1.97	0.46
9:W:37:ASN:C	9:W:37:ASN:HD22	2.19	0.46
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.10	0.45
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.65	0.45
2:B:113:ARG:NE	19:B:301:HOH:O	2.43	0.44
3:C:9:PHE:H	4:D:15:GLN:HE22	1.65	0.44
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.65	0.44
2:B:51:VAL:O	2:B:52:THR:C	2.55	0.43
4:R:125:LEU:N	19:R:301:HOH:O	2.50	0.43
2:P:51:VAL:CG1	2:P:51:VAL:O	2.59	0.43
3:Q:202:GLN:O	3:Q:202:GLN:CG	2.67	0.43
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.43
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.18	0.43
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.00	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.49	0.42
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.01	0.42
1:A:176:GLU:HG3	2:B:55:LEU:HD22	2.01	0.42
11:K:32:LYS:HB3	11:K:32:LYS:HE2	1.88	0.42
8:V:40:LYS:HE2	8:V:182:LYS:O	2.19	0.42
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.18	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.41
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.55	0.41
9:W:37:ASN:HD22	9:W:38:LYS:HG3	1.86	0.41
2:B:3:ARG:CZ	5:E:122:TYR:OH	2.68	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.03	0.41
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.18	0.41
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.41
11:K:209:ASN:ND2	19:K:401:HOH:O	2.47	0.41
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.03	0.40
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.03	0.40
9:I:37:ASN:HD22	9:I:38:LYS:HG3	1.86	0.40
8:V:3:ILE:HG22	8:V:16:ALA:HB2	2.03	0.40
7:G:73:VAL:HG12	7:G:133:THR:HB	2.04	0.40
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.40

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	248/250 (99%)	243 (98%)	5 (2%)	0	100	100
1	O	248/250 (99%)	243 (98%)	5 (2%)	0	100	100
2	B	242/258 (94%)	235 (97%)	6 (2%)	1 (0%)	34	66
2	P	242/258 (94%)	235 (97%)	7 (3%)	0	100	100
3	C	238/254 (94%)	235 (99%)	2 (1%)	1 (0%)	34	66
3	Q	238/254 (94%)	235 (99%)	2 (1%)	1 (0%)	34	66
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	34	66
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6284/6614 (95%)	6143 (98%)	137 (2%)	4 (0%)	51	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	52	THR
3	Q	204	GLY
3	C	204	GLY
13	a	229	GLY

### 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	209/209 (100%)	205 (98%)	4 (2%)	57	85
1	O	209/209 (100%)	205 (98%)	4 (2%)	57	85
2	B	203/216 (94%)	194 (96%)	9 (4%)	28	61
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	66
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	63
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30	63
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	64
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	64
5	E	190/193 (98%)	181 (95%)	9 (5%)	26	59
5	S	190/193 (98%)	181 (95%)	9 (5%)	26	59
6	F	201/239 (84%)	193 (96%)	8 (4%)	31	65
6	T	201/239 (84%)	192 (96%)	9 (4%)	27	60
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	206/210 (98%)	197 (96%)	9 (4%)	28	61
8	H	185/190 (97%)	178 (96%)	7 (4%)	33	67
8	V	185/190 (97%)	178 (96%)	7 (4%)	33	67
9	I	172/173 (99%)	169 (98%)	3 (2%)	60	87
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	92
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	82
10	X	173/175 (99%)	169 (98%)	4 (2%)	50	82
11	K	169/169 (100%)	162 (96%)	7 (4%)	30	64
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30	64
12	L	185/185 (100%)	179 (97%)	6 (3%)	39	73
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	62
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	70
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	74
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	74
All	All	5320/5540 (96%)	5130 (96%)	190 (4%)	35	69

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	52	THR
2	B	55	LEU
2	B	113	ARG
2	B	119	GLN
2	B	191	LEU
2	B	223	GLU
2	B	224	VAL
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS

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Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	99	ASN
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR

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Mol	Chain	Res	Type
8	H	68	LEU
8	H	120	ASP
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	90	LYS
10	J	99	GLN
11	K	9	GLN
11	K	53	GLN
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	130	SER
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	85	GLU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	36	ARG
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	2	THR
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	52	THR
2	P	55	LEU

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Mol	Chain	Res	Type
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	223	GLU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	99	ASN
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	214	TRP
6	T	221	ASN
6	T	240	GLN
7	U	83	ASN
7	U	115	LEU

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Mol	Chain	Res	Type
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	154	TYR
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	120	ASP
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	2	ASP
10	X	3	ILE
10	X	90	LYS
10	X	99	GLN
11	Y	9	GLN
11	Y	53	GLN
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	108	HIS
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	85	GLU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG

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Mol	Chain	Res	Type
14	b	9	LYS
14	b	36	ARG
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	92	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN

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Mol	Chain	Res	Type
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS

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Mol	Chain	Res	Type
4	R	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	22	GLN
8	V	30	ASN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	152	ASN
12	Z	153	GLN

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Mol	Chain	Res	Type
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	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 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
18	SO4	V	302	-	4,4,4	0.42	0	6,6,6	0.08	0
17	MES	H	301	-	12,12,12	2.00	3 (25%)	14,16,16	1.73	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	H	301	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	MES	C8-S	-5.41	1.69	1.77
17	H	301	MES	O1S-S	2.19	1.51	1.45
17	H	301	MES	O2S-S	2.13	1.51	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	MES	C6-C5-N4	4.45	116.85	110.10
17	H	301	MES	O3S-S-C8	2.69	110.12	105.77
17	H	301	MES	O2S-S-C8	2.61	110.06	106.92

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 ⓘ

### 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	250/250 (100%)	-0.36	8 (3%) 47 37	44, 57, 87, 107	0
1	O	250/250 (100%)	-0.25	6 (2%) 59 49	50, 67, 103, 126	0
2	B	244/258 (94%)	-0.24	11 (4%) 33 23	43, 62, 96, 114	0
2	P	244/258 (94%)	-0.22	8 (3%) 46 36	48, 65, 99, 117	0
3	C	240/254 (94%)	-0.14	10 (4%) 36 26	43, 66, 113, 156	0
3	Q	240/254 (94%)	0.11	17 (7%) 16 9	53, 80, 139, 183	0
4	D	235/260 (90%)	-0.35	5 (2%) 63 54	51, 67, 93, 129	0
4	R	235/260 (90%)	-0.23	6 (2%) 56 46	55, 71, 99, 138	0
5	E	231/234 (98%)	-0.18	3 (1%) 77 72	52, 70, 101, 118	0
5	S	231/234 (98%)	-0.10	7 (3%) 50 40	54, 76, 112, 132	0
6	F	243/288 (84%)	-0.37	5 (2%) 63 54	43, 64, 100, 123	0
6	T	243/288 (84%)	-0.28	6 (2%) 57 47	49, 73, 112, 142	0
7	G	241/252 (95%)	-0.47	1 (0%) 92 91	43, 57, 84, 115	0
7	U	241/252 (95%)	-0.34	5 (2%) 63 54	48, 62, 87, 119	0
8	H	226/232 (97%)	-0.41	7 (3%) 49 39	34, 51, 81, 148	0
8	V	226/232 (97%)	-0.30	7 (3%) 49 39	41, 55, 82, 151	0
9	I	204/205 (99%)	-0.58	1 (0%) 91 88	42, 52, 72, 86	0
9	W	204/205 (99%)	-0.57	2 (0%) 82 77	42, 55, 77, 89	0
10	J	195/198 (98%)	-0.50	3 (1%) 73 68	42, 56, 74, 89	0
10	X	195/198 (98%)	-0.43	3 (1%) 73 68	45, 58, 76, 100	0
11	K	212/212 (100%)	-0.54	0 100 100	44, 55, 73, 85	0
11	Y	212/212 (100%)	-0.51	0 100 100	45, 56, 78, 91	0
12	L	222/222 (100%)	-0.49	1 (0%) 91 88	43, 56, 82, 97	0
12	Z	222/222 (100%)	-0.49	1 (0%) 91 88	40, 55, 84, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	233/246 (94%)	-0.55	1 (0%) 92 91	39, 54, 75, 85	0
13	a	233/246 (94%)	-0.53	2 (0%) 84 80	41, 54, 72, 84	0
14	N	196/196 (100%)	-0.57	2 (1%) 82 77	37, 49, 73, 84	0
14	b	196/196 (100%)	-0.59	2 (1%) 82 77	38, 51, 74, 86	0
All	All	6344/6614 (95%)	-0.37	130 (2%) 65 56	34, 60, 98, 183	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	7.8
2	P	219	ALA	6.9
2	P	220	ASN	6.9
8	V	224	GLN	6.2
3	Q	49	THR	6.2
8	H	224	GLN	5.5
8	V	226	GLU	5.5
2	P	221	ASP	5.4
3	Q	236	GLN	5.1
8	V	221	CYS	5.1
2	B	221	ASP	4.9
8	V	222	ASP	4.6
10	X	194	ASP	4.5
3	Q	48	SER	4.4
12	L	174	TYR	4.4
7	U	242	GLN	4.3
2	B	220	ASN	4.2
5	E	202	ASP	4.2
3	Q	187	GLU	4.2
5	S	202	ASP	4.1
3	Q	55	THR	3.9
9	W	1	SER	3.9
8	V	223	ILE	3.8
14	b	195	GLN	3.8
3	Q	239	GLN	3.8
3	C	202	GLN	3.8
3	C	238	LYS	3.8
12	Z	174	TYR	3.7
8	H	226	GLU	3.6
3	Q	202	GLN	3.6
8	H	223	ILE	3.5
10	J	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
6	T	244	ASN	3.5
8	V	225	GLU	3.4
4	R	242	GLU	3.4
6	F	244	ASN	3.3
2	B	217	LYS	3.3
3	C	50	LEU	3.3
2	P	52	THR	3.2
3	C	206	LYS	3.2
10	X	1	MET	3.2
3	Q	206	LYS	3.2
3	Q	204	GLY	3.2
2	P	59	ASP	3.2
3	C	239	GLN	3.2
2	B	59	ASP	3.2
3	Q	240	GLU	3.2
3	Q	229	GLN	3.1
1	O	249	ALA	3.0
8	H	222	ASP	3.0
2	P	51	VAL	3.0
4	R	1	ASP	2.9
7	U	2	GLY	2.9
2	B	52	THR	2.9
1	A	249	ALA	2.9
4	R	241	ALA	2.9
5	S	173	ARG	2.9
3	C	216	ASP	2.8
6	T	180	PRO	2.8
9	I	1	SER	2.8
1	O	250	LEU	2.8
3	C	240	GLU	2.8
3	C	49	THR	2.8
7	U	181	LYS	2.7
6	T	178	HIS	2.7
4	D	242	GLU	2.7
2	B	51	VAL	2.7
3	C	236	GLN	2.7
13	M	47	ASP	2.6
3	Q	238	LYS	2.6
5	S	180	LYS	2.6
10	J	194	ASP	2.6
7	G	242	GLN	2.5
3	Q	52	LEU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	R	217	GLN	2.5
1	A	248	GLU	2.5
8	H	219	ASN	2.5
2	B	223	GLU	2.5
5	S	3	ASN	2.5
3	C	175	LYS	2.5
1	O	201	GLU	2.4
4	R	201	GLU	2.4
6	T	243	ILE	2.4
2	P	203	SER	2.4
14	N	195	GLN	2.4
14	b	105	LYS	2.4
10	J	193	ASP	2.4
3	Q	225	GLU	2.4
4	D	125	LEU	2.4
1	A	229	THR	2.4
2	B	50	LYS	2.4
5	E	201	ARG	2.4
7	U	241	GLU	2.4
1	O	231	LYS	2.4
7	U	222	ASP	2.4
13	a	171	GLN	2.4
3	Q	237	GLU	2.3
1	A	250	LEU	2.3
4	D	177	ASN	2.3
6	T	230	ASP	2.3
8	H	198	GLU	2.3
6	F	202	ASP	2.3
8	H	221	CYS	2.3
10	X	193	ASP	2.3
6	T	2	THR	2.3
1	O	50	LYS	2.3
14	N	105	LYS	2.3
1	A	52	SER	2.3
8	V	145	ASP	2.3
9	W	133	LYS	2.2
2	B	203	SER	2.2
2	B	242	GLY	2.2
13	a	1	THR	2.2
5	E	122	TYR	2.2
4	R	125	LEU	2.2
5	S	165	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
6	F	181	GLU	2.1
6	F	205	GLU	2.1
4	D	1	ASP	2.1
2	B	219	ALA	2.1
6	F	166	GLN	2.1
1	A	202	GLY	2.1
3	Q	205	ALA	2.1
1	A	231	LYS	2.1
2	P	50	LYS	2.1
4	D	2	ARG	2.1
1	O	52	SER	2.1
5	S	218	ASP	2.0
1	A	203	GLU	2.0
5	S	233	ILE	2.0

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	V	301	1/1	0.93	0.11	64,64,64,64	0
15	MG	Z	301	1/1	0.94	0.30	56,56,56,56	0
15	MG	I	301	1/1	0.94	0.23	69,69,69,69	0
17	MES	H	301	12/12	0.95	0.33	21,22,43,46	0
15	MG	G	301	1/1	0.95	0.06	45,45,45,45	0
18	SO4	V	302	5/5	0.96	0.28	66,68,72,81	0
16	CL	G	302	1/1	0.98	0.07	47,47,47,47	0
15	MG	K	301	1/1	0.99	0.08	52,52,52,52	0
15	MG	N	201	1/1	0.99	0.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	CL	U	301	1/1	0.99	0.10	50,50,50,50	0
15	MG	Y	301	1/1	0.99	0.04	58,58,58,58	0
15	MG	W	301	1/1	0.99	0.32	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.