wwPDB EM Validation Summary Report (i)

May 4, 2024 – 06:45 pm BST

PDB ID	:	6QM7
EMDB ID	:	EMD-4590
Title	:	Leishmania tarentolae proteasome 20S subunit complexed with GSK3494245
Authors	:	Rowland, P.; Goswami, P.
Deposited on	:	2019-02-01
Resolution	:	2.80 Å(reported)
Based on initial model	:	4R3O

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

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

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 49518 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 alpha1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	244	1857	1169	323	353	12	0	0
1	O	244	1857	1169	323	353	12	0	0

- Molecule 2 is a protein called Proteasome alpha2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	229	1754	1112	292	342	8	0	0
2	P	229	1754	1112	292	342	8	0	0

- Molecule 3 is a protein called Proteasome alpha3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	276	2195	1379	382	422	12	0	0
3	Q	276	2195	1379	382	422	12	0	0

- Molecule 4 is a protein called Proteasome alpha4 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	239	1873	1180	322	363	8	0	0
4	R	239	1873	1180	322	363	8	0	0

- Molecule 5 is a protein called Proteasome alpha5 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	229	1756	1094	302	347	13	0	0
5	S	229	1756	1094	302	347	13	0	0

- Molecule 6 is a protein called Proteasome alpha6 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	238	1869	1173	325	359	12	0	0
6	T	238	1869	1173	325	359	12	0	0

- Molecule 7 is a protein called Proteasome alpha7 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	228	1727	1077	306	334	10	0	0
7	U	228	1727	1077	306	334	10	0	0

- Molecule 8 is a protein called Proteasome beta1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	229	1710	1062	295	341	12	0	0
8	V	229	1710	1062	295	341	12	0	0

- Molecule 9 is a protein called Proteasome beta2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	219	1659	1037	292	318	12	0	0
9	W	219	1659	1037	292	318	12	0	0

- Molecule 10 is a protein called Proteasome beta3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	204	1557	980	259	302	16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	204	1557	980	259	302	16	0	0

- Molecule 11 is a protein called Proteasome beta4 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	206	1612	1012	280	304	16	0	0
11	Y	206	1612	1012	280	304	16	0	0

- Molecule 12 is a protein called Proteasome beta5 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	202	1579	998	277	297	7	0	0
12	Z	202	1579	998	277	297	7	0	0

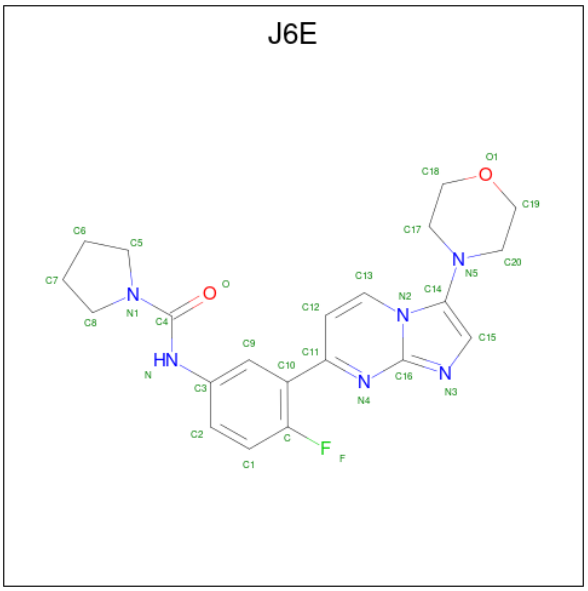
- Molecule 13 is a protein called Proteasome beta6 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	214	1702	1079	287	324	12	0	0
13	a	214	1702	1079	287	324	12	0	0

- Molecule 14 is a protein called Proteasome beta7 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	218	1712	1083	292	323	14	0	0
14	b	218	1712	1083	292	323	14	0	0

- Molecule 15 is {N}-[4-fluoranyl-3-(3-morpholin-4-ylimidazo[1,2-a]pyrimidin-7-yl)phenyl]pyrrolidine-1-carboxamide (three-letter code: J6E) (formula: $C_{21}H_{23}FN_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	F	N	O	0
			30	21	1	6	2	
15	Z	1	Total	C	F	N	O	0
			30	21	1	6	2	

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	A	9	Total	O	0
			9	9	
16	B	9	Total	O	0
			9	9	
16	C	8	Total	O	0
			8	8	
16	D	6	Total	O	0
			6	6	
16	E	8	Total	O	0
			8	8	
16	F	8	Total	O	0
			8	8	
16	G	12	Total	O	0
			12	12	
16	H	21	Total	O	0
			21	21	
16	I	7	Total	O	0
			7	7	
16	J	15	Total	O	0
			15	15	

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
16	K	9	9	9	0
			Total	O	
16	L	15	15	15	0
			Total	O	
16	M	13	13	13	0
			Total	O	
16	N	21	21	21	0
			Total	O	
16	O	11	11	11	0
			Total	O	
16	P	13	13	13	0
			Total	O	
16	Q	8	8	8	0
			Total	O	
16	R	9	9	9	0
			Total	O	
16	S	6	6	6	0
			Total	O	
16	T	8	8	8	0
			Total	O	
16	U	5	5	5	0
			Total	O	
16	V	19	19	19	0
			Total	O	
16	W	15	15	15	0
			Total	O	
16	X	23	23	23	0
			Total	O	
16	Y	8	8	8	0
			Total	O	
16	Z	17	17	17	0
			Total	O	
16	a	11	11	11	0
			Total	O	
16	b	20	20	20	0

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	J6E	L	4000	-	29,34,34	0.66	0	34,48,48	0.86	1 (2%)
15	J6E	Z	4000	-	29,34,34	0.64	0	34,48,48	0.74	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	J6E	L	4000	-	-	0/12/31/31	0/5/5/5
15	J6E	Z	4000	-	-	0/12/31/31	0/5/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	4000	J6E	C13-C12-C11	2.89	120.13	118.03
15	Z	4000	J6E	C13-C12-C11	2.71	120.00	118.03
15	Z	4000	J6E	C12-C13-N2	-2.07	118.09	120.66

There are no chirality outliers.

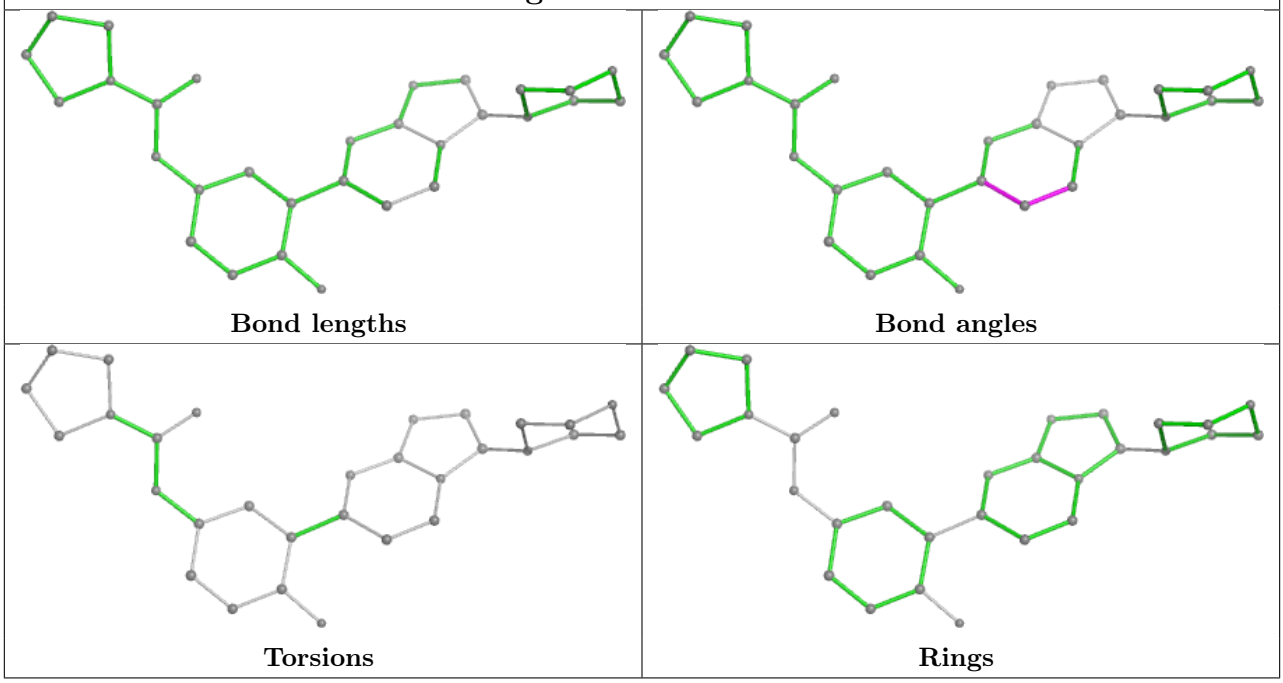
There are no torsion outliers.

There are no ring outliers.

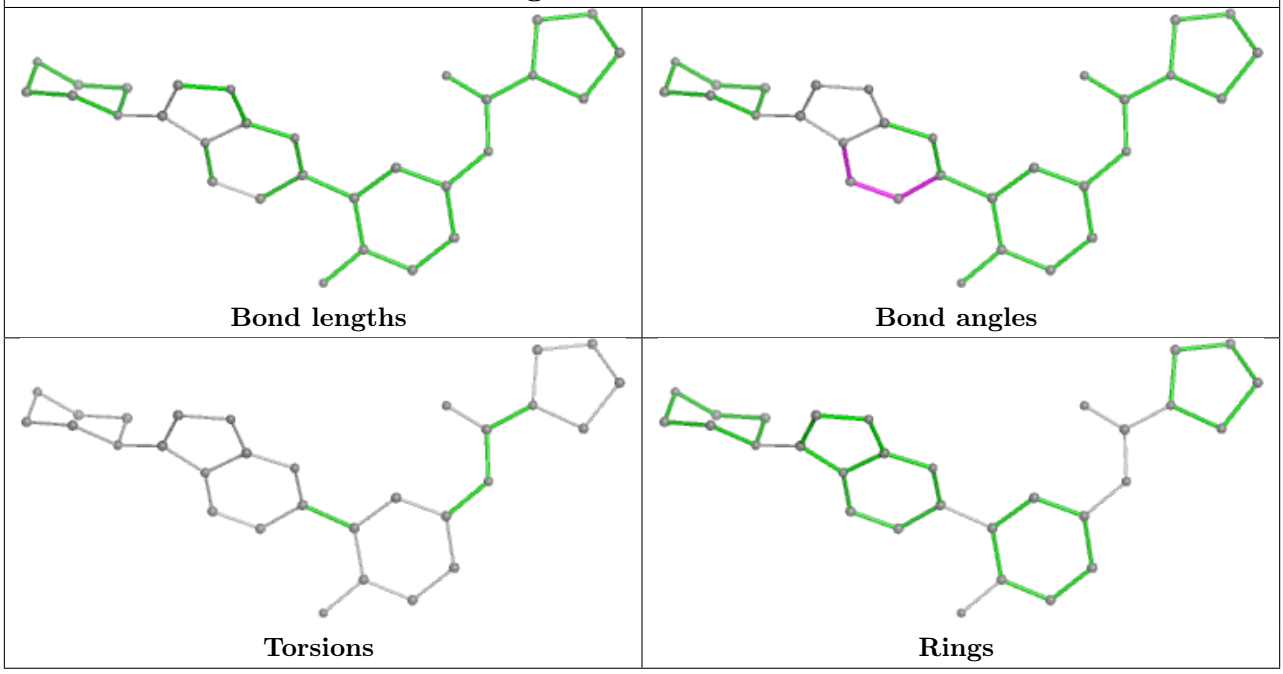
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand J6E L 4000



Ligand J6E Z 4000



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4590. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections (i)

This section was not generated.

5.2 Central slices (i)

This section was not generated.

5.3 Largest variance slices (i)

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

5.5 Orthogonal surface views (i)

This section was not generated.

5.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

6 Map analysis (i)

This section contains the results of statistical analysis of the map.

6.1 Map-value distribution (i)

This section was not generated.

6.2 Volume estimate versus contour level (i)

This section was not generated.

6.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit (i)

This section was not generated.