

wwPDB EM Validation Summary Report (i)

Jan 15, 2022 - 08:25 am GMT

PDB ID	:	7PXC
EMDB ID	:	EMD-13697
Title	:	Substrate-engaged mycobacterial Proteasome-associated ATPase in complex
		with open-gate $20S \text{ CP}$ - composite map (state A)
Authors	:	Jomaa, A.; Kavalchuk, M.; Weber-Ban, E.
Deposited on	:	2021-10-08
Resolution	:	3.84 Å(reported)
Based on initial model	:	5KWA

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

EMDB validation analysis	:	0.0.0.dev 97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 3.84 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain			
1	0	248	• 68%	16%	•	13%
1	2	248	72%	13%	•	13%
1	4	248	6 9%	15%	•	13%
1	6	248	72%	13%	•	13%
1	8	248	70%	14%	•	13%
1	Ι	248	63% 2	20%	•	14%
1	Κ	248	18%	19%	•	12%
1	0	248	69%	16%	•	13%



Mol	Chain	Length	Quality of c	chain	
1	Q	248	67%	16%	• 13%
1	Т	248	66%	18%	• 14%
1	v	210	19%	1070	1470
1	Λ	240	69%	16%	• 14%
1	Z	248	65%	20%	• 13%
1	d	248	82%		• 13%
1	f	248	82%		5% 13%
2	1	609	99%		
2	А	609	58%	18% •	23%
2	В	609	60%	18%	22%
2	С	609	59%	18%	23%
2	D	609	40%	16%	25%
2	E	609	11% 60%	18%	210/
2	F	600	13%	10%	2170
2	Г	009	61%	18%	21%
3	G	66	24%	74%	
4	Н	291	71%	•	24%
4	J	291	66%	10%	23%
4	L	291	67%	9%	24%
4	М	291	69%	7%	24%
4	Ν	291	69%	7%	24%
4	Р	291	68%	9%	23%
4	R	291	66%	10%	24%
4	S	291	• 69%	6% •	24%
4	U	291	71%	9%	20%
4	V	201	710/	50/	23%
1		201		570	2004
4	V W	291 291	71%	5%	23%



Mol	Chain	Length	Quality of chain						
4	Y	291	68%	8%	23%				
4	a	291	76%		• 23%				
4	b	291	74%	•	23%				



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 68808 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.

Mol	Chain	Residues		At	oms			AltConf	Trace			
1	0	215	Total	С	Ν	0	S	0	0			
	0	210	1658	1039	303	313	3	0	0			
1	2	215	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
		210	1658	1039	303	313	3	0	0			
1	4	215	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
	1	210	1658	1039	303	313	3	0	0			
1	6	215	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
1	0	210	1658	1039	303	313	3	0	0			
1	8	215	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
1	0	210	1658	1039	303	313	3	0	0			
1	т	214	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
1	-	-	T	T	214	1650	1033	302	312	3	0	0
1	K	217	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
1	11		1668	1044	305	316	3	0	0			
1	0	0 215	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
L	U	210	1658	1039	303	313	3	0	0			
1	0	215	Total	С	Ν	0	\mathbf{S}	0	0			
1	Q	210	1658	1039	303	313	3	0	0			
1	Т	914	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
1	T	214	1650	1033	302	312	3	0	0			
1	v	914	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0			
L	Λ	214	1650	1033	302	312	3	0	0			
1	7	215	Total	С	Ν	0	\mathbf{S}	0	0			
L		210	1658	1039	303	313	3	0	0			
1	d	215	Total	С	N	0	S	0	0			
	u	210	1658	1039	303	313	3		U			
1	f	215	Total	С	Ν	0	S	0	0			
	1	210	1658	1039	303	313	3		U			

• Molecule 1 is a protein called Proteasome subunit alpha.

• Molecule 2 is a protein called Proteasome-associated ATPase.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	1	5	Total C N O 42 28 6 8	0	0



Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
0	2 1	168	Total	С	Ν	0	S	0	0
	A	400	3665	2318	630	706	11	0	0
2	В	473	Total	С	Ν	Ο	\mathbf{S}	0	0
	D	475	3701	2338	635	717	11	0	0
9	C	471	Total	С	Ν	0	S	0	0
	U		3685	2326	634	714	11		0
0	Л	D 457	Total	С	Ν	0	S	0	0
	D		3584	2270	613	690	11	0	0
0	F	482	Total	С	Ν	0	S	0	0
	400	3775	2378	651	735	11	0	U	
9	9 F	402	Total	С	Ν	0	S	0	0
	Ľ	400	3773	2377	651	734	11	U	U

• Molecule 3 is a protein called Prokaryotic ubiquitin-like protein Pup.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	G	17	Total 112	C 62	N 23	O 26	S 1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
G	-1	GLY	-	expression tag	UNP P9WHN5	
G	0	SER	-	expression tag	UNP P9WHN5	

• Molecule 4 is a protein called Proteasome subunit beta.

Mol	Chain	Residues		At	oms			AltConf	Trace	
4	п	222	Total	С	Ν	0	S	0	0	
4	п		1636	1026	282	323	5	0	0	
4	т	222	Total	С	Ν	0	S	0	0	
4	1	223	1640	1028	283	324	5	0	0	
4	т	222	Total	С	Ν	0	S	0	0	
4			1636	1026	282	323	5	0		
4	м	м	222	Total	С	Ν	0	S	0	0
4	111		1636	1026	282	323	5	0	0	
4	N	າາາ	Total	С	Ν	0	S	0	0	
4	1 N		1636	1026	282	323	5	0	0	
4	D	<u> </u>	Total	С	Ν	0	S	0	0	
4	<u>4</u> Г	223	1640	1028	283	324	5	0	0	
4	A D	0 000	Total	С	Ν	0	S	0	0	
4	ц		1636	1026	282	323	5		0	



Mol	Chain	Residues		Atoms					Trace
4	q	າາາ	Total	С	Ν	0	S	0	0
4	C C		1636	1026	282	323	5	0	0
4	T	224	Total	С	Ν	0	S	0	0
4	U	234	1715	1072	295	343	5	0	0
4	V	222	Total	С	Ν	0	S	0	0
4	v	223	1640	1028	283	324	5	0	0
4	W/	224	Total	С	Ν	0	S	0	0
4	vv	234	1715	1072	295	343	5	0	0
4	V	222	Total	С	Ν	0	S	0	0
4	I	223	1640	1028	283	324	5	0	0
4		222	Total	С	Ν	0	S	0	0
4	a	223	1640	1028	283	324	5	0	0
4	h	222	Total	С	Ν	0	S	0	0
4	U	223	1640	1028	283	324	5		U

• Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
Б	Δ	1	Total	С	Ν	0	Р	0
5	A	L	31	10	5	13	3	0
Б	D	1	Total	С	Ν	0	Р	0
0	D	L	31	10	5	13	3	0
5	C	1	Total	С	Ν	0	Р	0
0	U	L	31	10	5	13	3	0
5	Б	1	Total	С	Ν	0	Р	0
0	E	L	31	10	5	13	3	0



Continued from previous page...

Mol	Chain	Residues		Atoms				
5	Б	1	Total	С	Ν	Ο	Р	0
5	Г		31	10	5	13	3	U

• Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
6	А	1	Total Mg 1 1	0
6	В	1	Total Mg 1 1	0
6	С	1	Total Mg 1 1	0
6	Е	1	Total Mg 1 1	0
6	F	1	Total Mg 1 1	0

• Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total 27	C 10	N 5	O 10	Р 2	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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



• Molecule 1: Proteasome subunit alpha

































PR0 GLU LEUA ASP ASP ASP ASP C21 C21 C21 C21 C22 C22 C22 C22 C22 C22	240 1240 1241 1241 1245 1245 1245 1255 1277 1277 1277	L290 L291 B316 V317 V317 B318 B318 B320 D321 D321 K326	N331 1332 1333 1333 1333 1333 1333 1339 1339
Last A360 A360 A360 A360 A365 B371 B374 B375 B375 B375 B375 B376 B376 B376 B376 B377 B377 B377 B377	V388 E389 E401 M408 M408 M419 M419 M4219 M4219	D422 R427 P428 R429 R429 R429 R429 R435 R435 R435 R435 R435 R435 R435 R435	D463 L464 A465 C469 V482 M486
Y4.87 A4.88 A4.89 A4.94 A4.94 A4.94 F4.96 F4.96 A5.01 A5.00	NS 14 NS 21 NS 21 NS 25 NS 26 NS 21 NS 21	V552 1553 1555 1555 1566 1561 1561 1563 1563 1568 1568	D669 W570 A571 R572 S574 C575 K577 K577 K577
E579 R5800 V832 V832 V832 V832 F584 F585 F586 F586 C5800 G5800 G5800 C58	ASP THR GLU BSER L605 L605 L605		
• Molecule 3: Prokaryotic ubiq	uitin-like protein Pup		
15% Chain G: 24% .	74%		_
G-1 SG-1 M1 E4 05 C11 C12 C12 C12 C12 C12 C12 C12 C12 C12	THR THR ALA ALA ALA ALA GLU CLU CLU CLU CLU CLU CLU CLU CLU CLU C	ASP LEU LEU LEU ASP ASP ASP ASP CLU CLU ASN ASN	OLU ASP PHE VAL ARG ARG AIA VAL CJA UAL CJA LYS
ALD GLN GLN			
• Molecule 4: Proteasome subt	mit beta		
Chain H:	71%	• 24%	-
MET THR PRO PRO PRO PRO ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	SER PHE ASP PHE ASP PHE LEU ARG GLN PHC GLU CLEU CLEU ALA ARA	SER ILE SER GLY GLY GLY PRO ALA GLY GLY GLN	LEU PRO GLY T301 1303 1303
R3 29 D3 30 D3 44 I3 45 R3 82 R3 82 E4 33 E4 33 E3 70 E3 70 E4 33 E4 34 E4 34 E4 E4 E4 E4 E4 E4 E4 E4 E4 E4 E4 E4 E4	88.22 GLY ALA ASP ASP PHE GLY GLY GLY GLY CLY CLY		
• Molecule 4: Proteasome subu	nit beta		
• Molecule 4: Proteasome subu Chain J:	nit beta	10% 23%	_
Molecule 4: Proteasome subu Chain J:	1988 HALL SALES AND SALES	10% 23% 8111 8111 8111 8111 8111 8111 8111 81	LEU PRO HIS GLY Y308
• Molecule 4: Proteasome subu Chain J: • 66	M388 M388 M388 M428 M488 M488 M488 M488 M488 M488 M488	E438 ISBR 38 10% 53% 118 118 1144 04175 114 111 11 111 11 111 11 111 11 111 11 111 11 111 11 111 11 111 11 111 11 11 11 11 12 11 13 11 14 11 14 11 14 11 14 11 14 11 14 11 14 11 14 11 14 11 14 11 14 11 15 11 16 11 17 11 18 11 19 11	E512 Y308 LEU 1497 PR0 PR0 B13 GLY F301 Y308
• Molecule 4: Proteasome subt Chain J: 666 1000 10	1435 1436	10% 23% 11% 24% 11%	LEU LEU 1497 PR0 1497 HIS R509 GLY GL T301 E512 Y308
 Molecule 4: Proteasome subt Molecule 4: Proteasome subt Molecule 4: Proteasome subt 	² ² ² ¹	10% 23% 10% 23% 10% 23% 10% 23% 11% 11% 11% 11% 11% 11% 11% 1	LEU LEU 14.97 PRO 14.97 H13 R509 1301 E512 Y308
• Molecule 4: Proteasome subu Chain J: $\mathbf{\hat{e}}$ $\hat{$	Init beta S%	10% 23% 23% 23% 23% 24%	1400 LEU 1497 PR0 1497 HR0 117 HS0 118 T301 118 Y308

MET TRP TRP PRO PRO PRO PRO PRO SER SER SER SER SER SER SER SER SER SER	LEU LEU SER SER SER PHE THR PHE LEU ARG GLA CLA CLA CLA CLA CLA CLA CLA CLA CLA C	SER ILE SER GLY GLY ALA PRO LEU	ALA GLY GLY ASP ALA ALA GLN CLU CLY GLY CLY V312 V312
8320 8320 1345 1345 1345 1345 1345 1345 1383 1383 1383 1383 1383 1424 1429 1429 1429 1429 1429	1431 1444 1444 1459 1459 1450 1450 1461 1473 1473 1473 1481 1488	V487 R488 G489 I490 I497 S508	E512 E512 E512 E521 E522 G12 FHR FHR FHR FHR FHR FHR FHR FHR FHR FHR
SX1 MT9 XT9			
• Molecule 4: Proteasome s	subunit beta		
Chain M:	69%	7%	24%
MET TRP TRP PRO PRO PRO PRO ASS SER SER SER SER SER SER SER SER SER S	LEU LEU SER SER SER SER THR THR THR THR THR CIU CIU CIU CIU CIU CIU CIU CIU CIU CIU	SER ILE SER GLY GLY ALA PRO LEU	ALA GLY GLY GLY GLY GLY CLEU CLEU CLEU CLEU CLEU CLEU CLEU CLEU
P309 P318 P318 P331 P331 P331 P331 P331 P331	Pd 13 Pd 13 A438 A438 A436 P456 P454 P456 P455 P456 P456 P456 P457 P453 P456 P456 P457	S522 GLY ALA ASP THR PHE CLY	SER ASP GLY CLU LYS
• Molecule 4: Proteasome s	subunit beta		
Chain N:	69%	7%	24%
MET THR THR PRO PRO PRO LEU ARG ARG CLU LEU SER SER SER SER CLU THR SER SER SER SER SER VAL	ASP LEU SER SER SER PHE PHE ASP ASP ASP ASP ASP ALA ALA ALA ALA ALA	SER ILE SER GLY GLY ALA PRO LEU	GLY GLY GLY GLY ASP GLN FRD FRD FRD FRD FRD FRD FRD FRD FRD FRD
R318 R318 8320 8320 8320 1330 1344 1345 8331 1345 8331 1345 1346 1346 1346 1346 1346 1346 1346 1346	1409 8412 8412 8412 8429 1431 1444 1444 1444 1444 1444 1444 144	GLY ALA ASP THR PHE GLY SER ASP	ULY CLIY CLIY CLIY CLIY
• Molecule 4: Proteasome s	subunit beta		
Chain P:	68%	9%	23%
MET THR TRP PRO PRO PRO LEU ASP SER SER SER SER SER SER SER SER SER ALA VAL	ASP LEU SER SER SER PHE ASP ASP ASP ASP ASP ASS ASP ASS ASS ASS	SER ILE SER GLY GLY ALA PRO LEU	d La GLY GLY GLY ASP GLN FRD FRD FRD FRD FRD FRD FRD FRD FRD FRD
V312 8320 8320 9330 V331 V331 V359 V359 V359 V359 L369 L369 L383 L383 L383	A425 A426 1429 1430 1431 1444 1444 1444 1446 1486 1486 1486 148	G489 1490 1497 8509 E512	6523 ALA ASP ASP ASP THR PHE CLY SSR ASP CLY CLY CLY CLY CLY CLY
• Molecule 4: Proteasome s	subunit beta		
Chain R:	66%	10%	24%
MET THR THR PRO PRO PRO PRO ASP ASS SER SER SER SER SER SER SER SER ALA VAL	ASP LEU SER SER PHE THR ASP ASP ASP ASP ASP ALA ALA ALA ALA ALA	SER ILE SER GLY GLY ALA PRO LEU	d La GLY GLY GLY ASP GLN FLA FLA FLS GLY F301 CSP
V312 V312 V331 V331 V331 V351 V351 V351 V351 C358 C358 C358 C358 C358 C358 C358 C358	1385 1385 1386 1439 1431 1431 1431 1431 1431 1434 1434	A475 D476 T481 L486 V487	R498 1490 1490 1497 1497 1497 8509 617 617 ALIA ALIA ALIA

WORLDWIDE PROTEIN DATA BANK

PHE GLY SER ASP GLY GLY GLY CLY LYS

• Molecule 4: Proteasome subunit beta

Chain S:	69%	6% •	24%
MET THR THR PRO PRO PRO LEU PRO PRO PRO CLEU SER SER SER SER SER CLE VAL ALA ALA ALA	SER SER PHE THR ASP PHE LEU LEU CLEU CLEU CLEU CLEU CLEU CLEU	ILE SER GLY GLY ALA PRO LLEU	GLY GLY GLY ALA ALA ALA GLN FLO FLO FLO FLO FLO FLO F100 F100 F100 F100 F100 F100 F100 F10
R3 18 R3 29 D3 30 D3 30 D3 36 C3 44 C3 44 C3 44 C3 44 C3 46 R3 70 R3 66 R3 70 R3 86 R3 70 R3 86 R3 70 R3 86 R3 70 R3 86 R3 70 R3 86 R3 70 R3 86 R3 86 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3	D413 D413 1429 1430 1430 1440 1446 1446 1465 1471	L513 S522 GLY ALA ASP THR	PHE CLY SER ASP ASP CLY CLY CLY LYS
• Molecule 4: Proteasome sub	ounit beta		
Chain U:	71%	9%	20%
MET THR THR PRO PRO LEU ARC ARC ARC ARC ARC ARC ARC ARC ARC ARC	SER SER PHE TTHR ASP PHE LEU ALA ALA CLU CLU CLU CLU CLU CLU SER SER	ILE SER GLY GLY ALA PRO LEU ALA	GLY CLY CLY ALA ALA GLN FRO FRO HTS GLY T301 V312
V313 M314 M329 M330	W429 N420 1431 1431 1432 E433 E433 E433 D456 D461 D461 D461 D461 D461 D461 D461 D476 D476	L486 V487 R488 G489 I490 I497	A524 D525 F527 F527 6528 5529 5529 5529 5530 6531 6532 6533 F533
• Molecule 4: Proteasome sub	ounit beta		
Chain V:	71%	5%	23%
MET THR THR PRO PRO PRO PRO PRO ASO ASO SER ASO SER ASO SER ASO VAL AVAL ASP	SER SER PHE TTRR ASP PHE LEU ARG CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ILE SER GLY GLY ALA PRO LEU ALA	GLY GLY GLY ASP ALA ALA CLN CLN CLN CLY CSC T301 T301 T303 T303 CSC T303 T303
P309 P335 P335 P338 P338 P338 P338 P345 P345 P345 P345 P345 P345 P345 P345	E432 E437 A437 L444 A438 A438 A444 A14 A14 A12 A14 A14 A14 A14 A14 A14 A18 A18 A18 A18 A18 A18 A18 A18 A18 A18	GLY GLV GLY	
• Molecule 4: Proteasome sub	ounit beta		
Chain W:	74%	6%	20%
MET TRP TRP PRO PRO PRO PRO PRO ASP SER SER SER SER SER SER SER SER SER SER	SER SER PHE THR THR ASP PHE LEU CLU CLU CLU CLU CLU CLU SER ASS SER	ILE SER GLY GLY ALA PRO LEU ALA	GLY GLY ASP ALA ALA CLU CLU FLU FLU FLU FLU FLU FLU FLU FLU FLU F
P309 D330 C344 C344 C344 C344 C344 C344 C346 C344 C346 C346	L444 M450 Y454 P465 L471 L513 d523 d523 d524 A524 A524 A524 A525 A524	6528 5529 5530 6531 6532 6532	K So 34
• Molecule 4: Proteasome sub	ounit beta		
Chain Y:	68%	8%	23%
MET TRP TRP PRO PRO PRO PRO PRO ASP ASS SER ASS SER ASS SER ASS SER ASS SER ASS LEU ASP LEU LEU LEU	SER PHE THR THR THR THR THR THR THR CILU CILU CILU CILU CILU CILU CILU CILU	ILE SER GLY GLY ALA PRO LEU ALA	GLY GLY ASP ASP GLN GLN FRO HIS GLN T301 V312 V312



8320 V331 V351 Y359 K368	L369 R382 L383 L383 L383 L388 L388 A426 A426 A426 A426	N430 1431 1434 1444 0459 0459 0461 0461	A475 T481 L486 L486 R487 R488 G489	1490 1497 E519	ALA ALA ASP ASP PHE GLY SER ASP	GLY GLU GLU
• Molecule 4:	Proteasome sub	unit beta				
Chain a:		76%		•	23%	_
MET THR TRP PRO LEU PRO ASP ASP LEU SER	ILE ASN ASN ASN SER SER SER SER CLY ALA ALA ASP LEU	SER PHE THR ASP PHE LEU LEU	AKG GLN PRO GLU LEU LEU PRO ALA	SER ILE SER GLY GLY ALA	LEU LEU GLY GLY ASP ALA GLN GLN	LEU PRO HIS GLY T301 L444
• Molecule 4:	Proteasome sub	unit beta				
Chain b:		74%		·	23%	-
MET THR TRP PRO LEU PRO ASP ASP LEU SER	ILE ASN SER SER SER SER CLY THR PRO ALA ASP ASP LEU	SER PHE THR ASP PHE LEU	AKG GLN PRO GLU LEU LEU PRO ALA	SER ILE SER GLY ALA	FRU LEU GLY GLY ASP ALA GLN GLN	LEU PRO GLY T301 P309
1345 8412 8412 8433 8433 1444 1444	E5 12 E5 12 ALA ALA ALA ASP PHE CLY ASP ASP ASP ASP	CLYS GLU				



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48054	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0216	Depositor
Map size (Å)	430.144, 430.144, 430.144	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.222, 1.222, 1.222	Depositor



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, ATP, ADP

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
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	0	0.42	0/1683	0.57	0/2274
1	2	0.41	0/1683	0.57	0/2274
1	4	0.41	0/1683	0.57	0/2274
1	6	0.42	0/1683	0.56	0/2274
1	8	0.43	0/1683	0.58	0/2274
1	Ι	0.36	0/1675	0.53	0/2263
1	Κ	0.35	0/1693	0.51	0/2287
1	0	0.35	0/1683	0.53	0/2274
1	Q	0.37	0/1683	0.53	0/2274
1	Т	0.36	0/1675	0.52	0/2263
1	Х	0.35	0/1675	0.52	0/2263
1	Ζ	0.38	0/1683	0.54	0/2274
1	d	0.42	0/1683	0.59	0/2274
1	f	0.46	0/1683	0.59	0/2274
2	1	0.57	0/42	0.55	0/54
2	А	0.27	0/3724	0.43	0/5033
2	В	0.27	0/3761	0.42	0/5085
2	С	0.30	0/3745	0.44	0/5062
2	D	0.34	0/3643	0.47	0/4923
2	Е	0.30	0/3837	0.44	0/5189
2	F	0.29	0/3835	0.43	0/5186
3	G	0.23	0/111	0.44	0/143
4	Н	0.38	0/1660	0.58	0/2251
4	J	0.39	0/1664	0.58	0/2256
4	L	0.40	0/1660	0.59	0/2251
4	М	0.38	0/1660	0.57	0/2251
4	N	0.39	0/1660	0.58	0/2251
4	Р	0.39	0/1664	0.59	0/2256
4	R	0.39	0/1660	0.58	0/2251
4	S	0.38	0/1660	0.58	0/2251
4	U	0.40	0/1740	0.58	0/2357
4	V	0.39	0/1664	0.58	0/2256



Mal	Chain	Chain Bond lengths			angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
4	W	0.38	0/1740	0.56	0/2357
4	Y	0.39	0/1664	0.60	0/2256
4	а	0.40	0/1664	0.59	0/2256
4	b	0.38	0/1664	0.57	0/2256
All	All	0.36	0/69670	0.53	0/94247

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	378	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1658	0	1659	46	0
1	2	1658	0	1659	28	0
1	4	1658	0	1659	51	0
1	6	1658	0	1659	19	0
1	8	1658	0	1659	27	0
1	Ι	1650	0	1648	35	0
1	K	1668	0	1667	29	0
1	0	1658	0	1659	24	0
1	Q	1658	0	1659	27	0
1	Т	1650	0	1648	30	0



Conti	nuea fron	<i>i previous</i>	page	1	1	
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Х	1650	0	1648	26	0
1	Z	1658	0	1659	31	0
1	d	1658	0	1659	0	0
1	f	1658	0	1659	0	0
2	1	42	0	41	22	0
2	А	3665	0	3691	79	0
2	В	3701	0	3721	75	0
2	С	3685	0	3700	65	0
2	D	3584	0	3605	86	0
2	Е	3775	0	3779	83	0
2	F	3773	0	3777	86	0
3	G	112	0	102	2	0
4	Н	1636	0	1625	8	0
4	J	1640	0	1628	17	0
4	L	1636	0	1625	14	0
4	М	1636	0	1625	11	0
4	N	1636	0	1625	10	0
4	Р	1640	0	1628	13	0
4	R	1636	0	1625	16	0
4	S	1636	0	1625	12	0
4	U	1715	0	1690	16	0
4	V	1640	0	1628	8	0
4	W	1715	0	1690	9	0
4	Y	1640	0	1628	13	0
4	a	1640	0	1628	0	0
4	b	1640	0	1628	0	0
5	А	31	0	12	3	0
5	В	31	0	12	4	0
5	С	31	0	12	4	0
5	Е	31	0	12	5	0
5	F	31	0	12	2	0
6	А	1	0	0	0	0
6	В	1	0	0	0	0
6	C	1	0	0	0	0
6	Е	1	0	0	0	0
6	F	1	0	0	0	0
7	D	27	0	12	1	0
All	All	68808	0	68587	911	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 911 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)
2:1:605:LEU:CD2	1:4:144:ASP:HB2	1.53	1.39
2:1:605:LEU:HD23	1:4:144:ASP:CB	1.68	1.22
1:2:13:MET:SD	2:A:605:LEU:HG	1.84	1.15
2:1:605:LEU:CD2	1:4:144:ASP:CB	2.22	1.13
2:1:605:LEU:HD23	1:4:144:ASP:HB2	1.13	1.10

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 PDB entries followed by that with respect to all EM entries.

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	Perce	entiles
1	0	211/248~(85%)	202 (96%)	9 (4%)	0	100	100
1	2	211/248~(85%)	203 (96%)	8 (4%)	0	100	100
1	4	211/248~(85%)	203~(96%)	8 (4%)	0	100	100
1	6	211/248~(85%)	204 (97%)	7 (3%)	0	100	100
1	8	211/248~(85%)	201~(95%)	10 (5%)	0	100	100
1	Ι	210/248~(85%)	203 (97%)	7 (3%)	0	100	100
1	K	213/248~(86%)	205~(96%)	8 (4%)	0	100	100
1	Ο	211/248~(85%)	205~(97%)	6 (3%)	0	100	100
1	Q	211/248~(85%)	204 (97%)	7 (3%)	0	100	100
1	Т	210/248~(85%)	202 (96%)	8 (4%)	0	100	100
1	Х	210/248~(85%)	204 (97%)	6 (3%)	0	100	100
1	Z	211/248~(85%)	204 (97%)	7 (3%)	0	100	100
1	d	211/248~(85%)	203~(96%)	8 (4%)	0	100	100
1	f	211/248~(85%)	202 (96%)	9 (4%)	0	100	100
2	1	3/609~(0%)	2(67%)	1 (33%)	0	100	100
2	А	458/609~(75%)	442 (96%)	15 (3%)	1 (0%)	47	78



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	В	465/609~(76%)	452 (97%)	13 (3%)	0	100	100
2	С	463/609~(76%)	451 (97%)	12 (3%)	0	100	100
2	D	447/609 (73%)	426 (95%)	17 (4%)	4 (1%)	17	53
2	Е	477/609~(78%)	457 (96%)	20 (4%)	0	100	100
2	F	477/609 (78%)	460 (96%)	16 (3%)	1 (0%)	47	78
3	G	15/66~(23%)	15 (100%)	0	0	100	100
4	Н	220/291~(76%)	211 (96%)	9 (4%)	0	100	100
4	J	221/291~(76%)	211 (96%)	10 (4%)	0	100	100
4	L	220/291~(76%)	209 (95%)	11 (5%)	0	100	100
4	М	220/291~(76%)	211 (96%)	8 (4%)	1 (0%)	29	66
4	Ν	220/291~(76%)	212 (96%)	7 (3%)	1 (0%)	29	66
4	Р	221/291~(76%)	210 (95%)	11 (5%)	0	100	100
4	R	220/291~(76%)	210 (96%)	10 (4%)	0	100	100
4	S	220/291~(76%)	213 (97%)	6 (3%)	1 (0%)	29	66
4	U	232/291~(80%)	221 (95%)	11 (5%)	0	100	100
4	V	221/291~(76%)	214 (97%)	6 (3%)	1 (0%)	29	66
4	W	232/291~(80%)	225 (97%)	6 (3%)	1 (0%)	34	70
4	Y	221/291~(76%)	210 (95%)	11 (5%)	0	100	100
4	a	221/291~(76%)	210 (95%)	11 (5%)	0	100	100
4	b	221/291 (76%)	214 (97%)	6 (3%)	1 (0%)	29	66
All	All	8868/11875 (75%)	8531 (96%)	325 (4%)	12 (0%)	54	83

Continued from previous page...

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	А	505	LYS
2	D	342	VAL
2	F	378	ARG
2	D	295	PRO
2	D	297	CYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM



entries.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	0	165/192~(86%)	157~(95%)	8 (5%)	25	55
1	2	165/192~(86%)	159~(96%)	6 (4%)	35	62
1	4	165/192~(86%)	157 (95%)	8 (5%)	25	55
1	6	165/192~(86%)	156 (94%)	9 (6%)	21	53
1	8	165/192~(86%)	156 (94%)	9 (6%)	21	53
1	Ι	164/192~(85%)	154 (94%)	10 (6%)	18	50
1	K	166/192~(86%)	158 (95%)	8 (5%)	25	55
1	О	165/192~(86%)	155 (94%)	10 (6%)	18	50
1	Q	165/192~(86%)	154 (93%)	11 (7%)	16	47
1	Т	164/192~(85%)	156 (95%)	8 (5%)	25	55
1	Х	164/192~(85%)	159 (97%)	5 (3%)	41	66
1	Z	165/192~(86%)	156 (94%)	9 (6%)	21	53
1	d	165/192~(86%)	154 (93%)	11 (7%)	16	47
1	f	165/192~(86%)	153 (93%)	12 (7%)	14	44
2	1	4/511 (1%)	4 (100%)	0	100	100
2	А	397/511~(78%)	389~(98%)	8 (2%)	55	74
2	В	402/511 (79%)	394 (98%)	8 (2%)	55	74
2	С	400/511 (78%)	388~(97%)	12 (3%)	41	66
2	D	$388/511\ (76\%)$	377 (97%)	11 (3%)	43	67
2	Е	409/511 (80%)	398~(97%)	11 (3%)	44	68
2	F	408/511 (80%)	403 (99%)	5 (1%)	71	84
3	G	10/50~(20%)	10 (100%)	0	100	100
4	Н	164/217~(76%)	161 (98%)	3 (2%)	59	77
4	J	164/217~(76%)	158 (96%)	6 (4%)	34	61
4	L	164/217~(76%)	161 (98%)	3 (2%)	59	77
4	М	164/217~(76%)	160 (98%)	4 (2%)	49	71
4	Ν	164/217~(76%)	160 (98%)	4 (2%)	49	71
4	Р	164/217~(76%)	159 (97%)	5 (3%)	41	66
4	R	164/217~(76%)	160 (98%)	4 (2%)	49	71

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	Perce	ntiles
4	S	164/217~(76%)	159~(97%)	5(3%)	41	66
4	U	171/217~(79%)	166~(97%)	5(3%)	42	66
4	V	164/217~(76%)	161 (98%)	3~(2%)	59	77
4	W	171/217~(79%)	167~(98%)	4 (2%)	50	71
4	Y	164/217~(76%)	161 (98%)	3~(2%)	59	77
4	a	164/217~(76%)	161 (98%)	3~(2%)	59	77
4	b	164/217~(76%)	158 (96%)	6 (4%)	34	61
All	All	7036/9353~(75%)	6799(97%)	237 (3%)	40	64

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Κ	26	ARG
1	d	144	ASP
4	Р	330	ASP
1	d	73	ASN
1	f	234	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such side chains are listed below:

Mol	Chain	Res	Type
4	R	430	ASN
4	Y	456	GLN
4	S	456	GLN
1	Х	11	GLN
1	Z	174	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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).

Mal	Turne	Chain	Res	s Link	Bo	ond leng	$_{\rm ths}$	Bond angles		
Moi Type	туре				Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	ATP	А	701	6	26,33,33	0.93	1 (3%)	31,52,52	1.54	5 (16%)
5	ATP	F	701	6	26,33,33	0.92	1 (3%)	31,52,52	1.60	5 (16%)
5	ATP	В	701	6	26,33,33	0.93	1 (3%)	31,52,52	1.58	5 (16%)
7	ADP	D	701	-	24,29,29	0.66	0	29,45,45	0.83	1 (3%)
5	ATP	Е	701	6	26,33,33	0.92	1 (3%)	31,52,52	1.62	5 (16%)
5	ATP	С	701	6	26,33,33	0.91	1 (3%)	31,52,52	1.48	5 (16%)

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
5	ATP	А	701	6	-	0/18/38/38	0/3/3/3
5	ATP	F	701	6	-	0/18/38/38	0/3/3/3
5	ATP	В	701	6	-	0/18/38/38	0/3/3/3
7	ADP	D	701	-	-	2/12/32/32	0/3/3/3
5	ATP	Е	701	6	-	0/18/38/38	0/3/3/3
5	ATP	С	701	6	-	0/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	А	701	ATP	C5-C4	2.49	1.47	1.40
5	F	701	ATP	C5-C4	2.47	1.47	1.40



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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\operatorname{\AA})$			
5	В	701	ATP	C5-C4	2.46	1.47	1.40			
5	Е	701	ATP	C5-C4	2.44	1.47	1.40			
5	С	701	ATP	C5-C4	2.44	1.47	1.40			

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Е	701	ATP	PA-O3A-PB	-4.42	117.65	132.83
5	Е	701	ATP	PB-O3B-PG	-4.28	118.14	132.83
5	F	701	ATP	PA-O3A-PB	-4.17	118.50	132.83
5	В	701	ATP	PA-O3A-PB	-4.16	118.55	132.83
5	В	701	ATP	PB-O3B-PG	-4.14	118.61	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	701	ADP	C3'-C4'-C5'-O5'
7	D	701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	701	ATP	3	0
5	F	701	ATP	2	0
5	В	701	ATP	4	0
7	D	701	ADP	1	0
5	Е	701	ATP	5	0
5	С	701	ATP	4	0

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.



















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 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13697. 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.

Orthogonal projections (i) 6.1

6.1.1Primary map



The images above show the map projected in three orthogonal directions.

6.2Central slices (i)

6.2.1Primary map



X Index: 176

Y Index: 176



The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 155

Y Index: 152

Z Index: 182

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 393 nm^3 ; this corresponds to an approximate mass of 355 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.260 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13697 and PDB model 7PXC. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

