



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:19 PM BST

PDB ID : 5FTJ  
EMDB ID: : EMD-3295  
Title : Cryo-EM structure of human p97 bound to UPCDC30245 inhibitor  
Authors : Banerjee, S.; Bartesaghi, A.; Merk, A.; Rao, P.; Bulfer, S.L.; Yan, Y.; Green, N.; Mroczkowski, B.; Neitz, R.J.; Wipf, P.; Falconieri, V.; Deshaies, R.J.; Milne, J.L.S.; Hury, D.; Arkin, M.; Subramaniam, S.  
Deposited on : 2016-01-14  
Resolution : 2.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

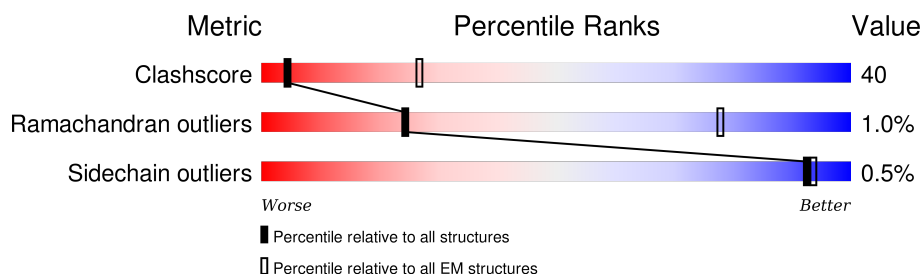
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.30 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	806	50% 39% • 10%
1	B	806	48% 40% • 10%
1	C	806	49% 39% • 10%
1	D	806	49% 40% • 10%
1	E	806	49% 40% • 10%
1	F	806	49% 39% • 10%

## 2 Entry composition [i](#)

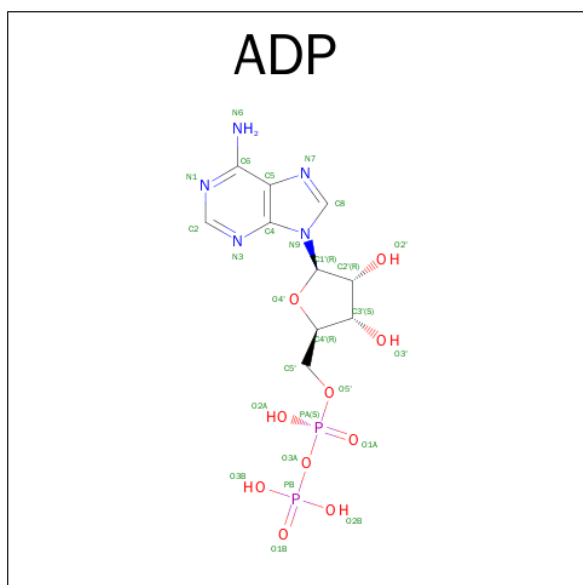
There are 4 unique types of molecules in this entry. The entry contains 34602 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE.

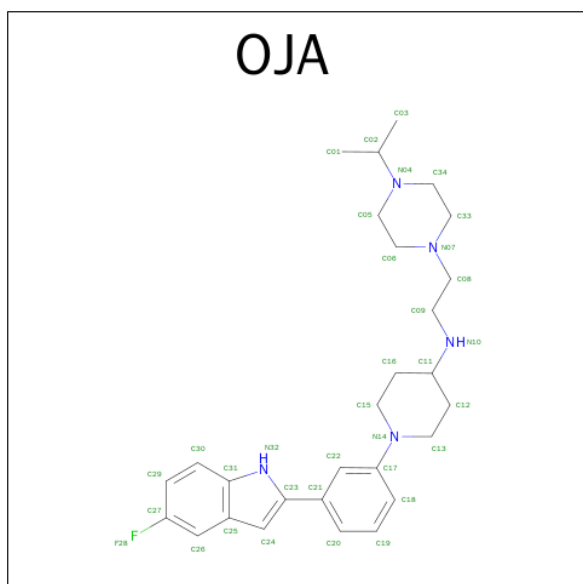
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	B	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	C	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	D	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	E	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	F	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	E	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	F	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	F	1	Total	C	N	O	P	0
			54	20	10	20	4	

- Molecule 3 is 1-(3-(5-FLUORO-1H-INDOL-2-YL)PHENYL)PIPERIDIN-4-YL)(2-(4-ISO  
PROPYL-PIPERAZIN-1-YL)ETHYL)-CARBAMATE (three-letter code: OJA) (formula:  
 $C_{28}H_{38}FN_5$ ).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	F	N	0
			34	28	1	5	
3	B	1	Total	C	F	N	0
			34	28	1	5	
3	C	1	Total	C	F	N	0
			34	28	1	5	
3	D	1	Total	C	F	N	0
			34	28	1	5	
3	E	1	Total	C	F	N	0
			34	28	1	5	
3	F	1	Total	C	F	N	0
			34	28	1	5	

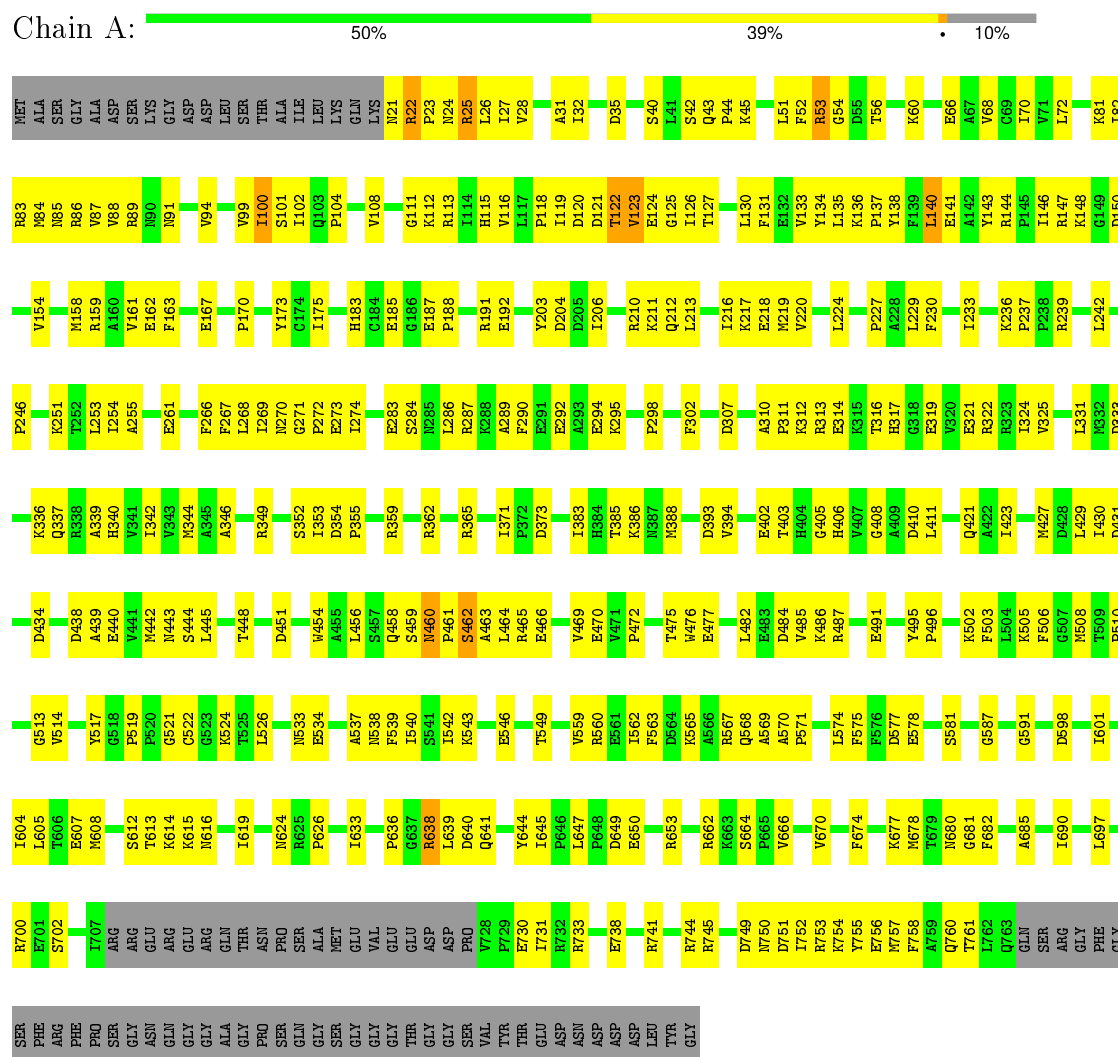
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	20	Total	O	0
			20	20	
4	B	20	Total	O	0
			20	20	
4	C	20	Total	O	0
			20	20	
4	D	20	Total	O	0
			20	20	
4	E	20	Total	O	0
			20	20	
4	F	20	Total	O	0
			20	20	

### 3 Residue-property plots

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. 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. 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: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



- Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

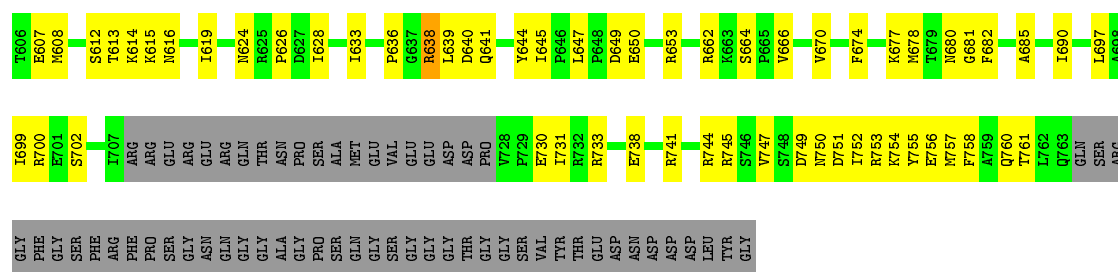


R83	G149	Y244	D333	D428	L504	D598	F682	M757	R83	G149	Y244	D333	D428	L504	D598	F682	M757
R84	D150	G245	K336	L429	K505	D598	A685	F759	R84	D150	G245	K336	L429	K505	D598	A685	F759
R85	V154	P246	Q337	T430	F506	I601	I680	Q760	R85	V154	P246	Q337	T430	F506	I601	I680	Q760
R86	M158	K251	R338	D431	P510	I604	I690	T761	R86	M158	K251	R338	D431	P510	I604	I690	T761
R87	M159	T252	A339	D434	G513	L605	G681	L762	R87	M159	T252	A339	D434	G513	L605	G681	L762
R88	A160	L253	R340	D438	V514	T606	Q692	Q763	R88	A160	L253	R340	D438	V514	T606	Q692	Q763
R89	R159	A255	R341	D439	Y517	M608	L697	GLN	R89	R159	A255	R341	D439	Y517	M608	L697	GLN
R90	V161	E261	F343	A439	G518	P519	A698	ARG	R90	V161	E261	F343	A439	G518	P519	A698	ARG
R91	E162	F267	M344	V441	P519	T613	L699	GLY	R91	E162	F267	M344	V441	P519	T613	L699	GLY
R92	F163	L268	A345	N442	G521	K614	R700	PHE	R92	F163	L268	A345	N442	G521	K614	R700	PHE
R93	E167	L269	A346	N443	G522	K615	S702	GLY	R93	E167	L269	A346	N443	G522	K615	S702	GLY
Y94	P170	L270	R349	N444	G523	N616	I707	ARG	Y94	P170	L270	R349	N444	G523	N616	I707	ARG
D98	P170	L268	R349	N444	G523	N616	I707	ARG	D98	P170	L268	R349	N444	G523	N616	I707	ARG
Y99	P170	L268	R349	N444	G523	N616	I707	ARG	Y99	P170	L268	R349	N444	G523	N616	I707	ARG
I100	Y173	N270	S351	N445	K524	I619	ARG	GLY	I100	Y173	N270	S351	N445	K524	I619	ARG	GLY
S101	G174	G271	S352	N446	T525	I624	GLY	GLN	S101	G174	G271	S352	N446	T525	I624	GLY	GLN
I102	I175	P272	I353	T448	L526	N624	GLY	GLY	I102	I175	P272	I353	T448	L526	N624	GLY	GLY
Q103	H183	L274	P395	D451	N533	I625	GLY	GLY	Q103	H183	L274	P395	D451	N533	I625	GLY	GLY
P104	C184	E283	R359	N454	E534	P626	GLY	GLY	P104	C184	E283	R359	N454	E534	P626	GLY	GLY
V108	E185	S284	R359	N454	E534	P626	GLY	GLY	V108	E185	S284	R359	N454	E534	P626	GLY	GLY
G111	G186	N285	R362	L455	A537	D630	THR	ALA	G111	G186	N285	R362	L455	A537	D630	THR	ALA
K112	E187	N285	R362	L455	A537	D630	THR	ALA	K112	E187	N285	R362	L455	A537	D630	THR	ALA
R113	P188	L286	R365	Q458	F539	A632	PRO	GLY	R113	P188	L286	R365	Q458	F539	A632	PRO	GLY
I114	R191	L287	R365	Q458	F539	A632	PRO	GLY	I114	R191	L287	R365	Q458	F539	A632	PRO	GLY
H115	E192	K288	R365	Q458	F539	A632	PRO	GLY	H115	E192	K288	R365	Q458	F539	A632	PRO	GLY
V116	E192	F290	I371	N460	S541	I633	ALA	GLY	V116	E192	F290	I371	N460	S541	I633	ALA	GLY
L117	Y203	A290	I371	N460	S541	I633	ALA	GLY	L117	Y203	A290	I371	N460	S541	I633	ALA	GLY
P118	D204	F290	I371	N460	S541	I633	ALA	GLY	P118	D204	F290	I371	N460	S541	I633	ALA	GLY
I119	D204	F290	I371	N460	S541	I633	ALA	GLY	I119	D204	F290	I371	N460	S541	I633	ALA	GLY
D120	D204	F290	I371	N460	S541	I633	ALA	GLY	D120	D204	F290	I371	N460	S541	I633	ALA	GLY
D121	I206	A292	I383	L464	T549	D640	GLY	GLY	D121	I206	A292	I383	L464	T549	D640	GLY	GLY
T122	K210	E293	T385	L466	T549	D640	GLY	GLY	T122	K210	E293	T385	L466	T549	D640	GLY	GLY
V123	K211	E293	T385	L466	T549	D640	GLY	GLY	V123	K211	E293	T385	L466	T549	D640	GLY	GLY
E124	Q212	A293	T385	L466	T549	D640	GLY	GLY	E124	Q212	A293	T385	L466	T549	D640	GLY	GLY
G125	L213	K295	T385	L466	T549	D640	GLY	GLY	G125	L213	K295	T385	L466	T549	D640	GLY	GLY
I126	K217	P298	T385	L466	T549	D640	GLY	GLY	I126	K217	P298	T385	L466	T549	D640	GLY	GLY
T127	K217	P298	T385	L466	T549	D640	GLY	GLY	T127	K217	P298	T385	L466	T549	D640	GLY	GLY
L130	E218	F302	D393	T475	V559	I645	PRO	GLY	L130	E218	F302	D393	T475	V559	I645	PRO	GLY
F131	M219	D307	D393	T475	V559	I645	PRO	GLY	F131	M219	D307	D393	T475	V559	I645	PRO	GLY
E132	L224	A310	E402	G480	Q567	R653	E738	ASN	E132	L224	A310	E402	G480	Q567	R653	E738	ASN
V133	P311	P311	E402	G480	Q567	R653	E738	ASN	V133	P311	P311	E402	G480	Q567	R653	E738	ASN
Y134	K312	K312	E402	G480	Q567	R653	E738	ASN	Y134	K312	K312	E402	G480	Q567	R653	E738	ASN
L135	P227	R313	G405	L482	A569	R662	R741	ASP	L135	P227	R313	G405	L482	A569	R662	R741	ASP
K136	P227	E314	G405	L482	A569	R662	R741	ASP	K136	P227	E314	G405	L482	A569	R662	R741	ASP
P137	A228	K315	G407	E483	P571	S664	R744	LEU	P137	A228	K315	G407	E483	P571	S664	R744	LEU
P138	L229	T316	V408	D484	L574	P665	R745	THR	P138	L229	T316	V408	D484	L574	P665	R745	THR
F139	F230	E319	D410	V485	L574	P665	R745	THR	F139	F230	E319	D410	V485	L574	P665	R745	THR
L140	I233	F320	D410	V485	L574	P665	R745	THR	L140	I233	F320	D410	V485	L574	P665	R745	THR
E141	E321	V320	L411	K487	F575	V670	S747	GLY	E141	E321	V320	L411	K487	F575	V670	S747	GLY
A142	E321	F320	L411	K487	F575	V670	S747	GLY	A142	E321	F320	L411	K487	F575	V670	S747	GLY
Y143	K236	R322	L414	E491	D577	F674	D749	GLY	Y143	K236	R322	L414	E491	D577	F674	D749	GLY
R144	P237	R322	L414	E491	D577	F674	D749	GLY	R144	P237	R322	L414	E491	D577	F674	D749	GLY
P145	P237	R322	L414	E491	D577	F674	D749	GLY	P145	P237	R322	L414	E491	D577	F674	D749	GLY
I146	P238	R323	L414	E491	D577	F674	D749	GLY	I146	P238	R323	L414	E491	D577	F674	D749	GLY
L147	R239	R323	L414	E491	D577	F674	D749	GLY	L147	R239	R323	L414	E491	D577	F674	D749	GLY
K148	L242	R332	L414	E491	D577	F674	D749	GLY	K148	L242	R332	L414	E491	D577	F674	D749	GLY

• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

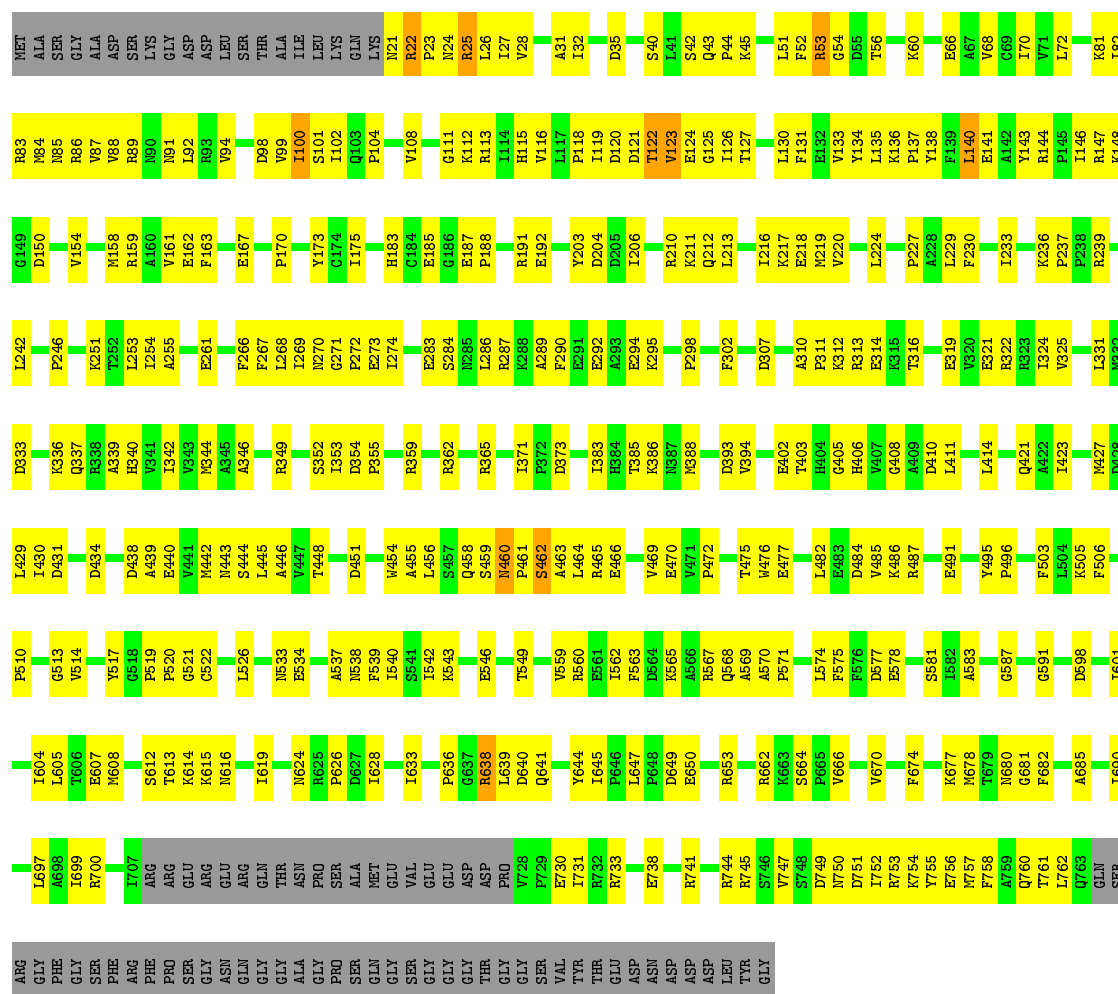
Chain C:  49% 39% 10%

MET	R81	G149	P246	K336	D434	V514		R81	G149	P246	K336	D434	V514
ALA	R82	D150	K251	Q337	D438	Y517		R82	D150	K251	Q337	D438	Y517
SER	R83	V154	T252	A339	A439	G518		R83	V154	T252	A339	A439	G518
GLY	R84	M158	L254	R340	P520	P519		R84	M158	L254	R340	P520	P519
ALA	R85	R159	I254	E441	G521	G522		R85	R159	I254	E441	G521	G522
ASP	R86	A160	A255	V441	C521	C522		R86	A160	A255	V441	C521	C522
SER	R87	E261	E261	M442	L526	L526		R87	E261	E261	M442	L526	L526
LYS	R88	F163	F163	S444	N533	N533		R88	F163	F163	S444	N533	N533
GLY	R89	E162	F266	L445	E534	E534		R89	E162	F266	L445	E534	E534
ASP	R90	E167	F267	V447	A537	A537		R90	E167	F267	V447	A537	A537
LEU	R91	E167	L268	T448	P539	P539		R91	E167	L268	T448	P539	P539
SER	R92	P170	N270	G271	I540	I540		R92	P170	N270	G271	I540	I540
THR	R93	P170	G271	I540	S541	S541		R93	P170	G271	I540	S541	S541
ALA	R94	P170	G271	I540	L456	L456		R94	P170	G271	I540	L456	L456
LEU	R95	E167	L274	H183	S457	S457		R95	E167	L274	H183	S457	S457
LYS	R96	E167	L274	H183	S457	S457		R96	E167	L274	H183	S457	S457
LYS	R97	E167	L274	H183	S457	S457		R97	E167	L274	H183	S457	S457
N21	R98	E167	L274	H183	S457	S457		R98	E167	L274	H183	S457	S457
R22	R99	E167	L274	H183	S457	S457		R99	E167	L274	H183	S457	S457
P23	R100	E167	L274	H183	S457	S457		R100	E167	L274	H183	S457	S457
N24	R101	E167	L274	H183	S457	S457		R101	E167	L274	H183	S457	S457
R25	R102	E167	L274	H183	S457	S457		R102	E167	L274	H183	S457	S457
L26	R103	E167	L274	H183	S457	S457		R103	E167	L274	H183	S457	S457
I27	R104	E167	L274	H183	S457	S457		R104	E167	L274	H183	S457	S457
V28	R105	E167	L274	H183	S457	S457		R105	E167	L274	H183	S457	S457
A31	R106	E167	L274	H183	S457	S457		R106	E167	L274	H183	S457	S457
I32	R107	E167	L274	H183	S457	S457		R107	E167	L274	H183	S457	S457
D35	R108	E167	L274	H183	S457	S457		R108	E167	L274	H183	S457	S457
V38	R109	E167	L274	H183	S457	S457		R109	E167	L274	H183	S457	S457
V39	R110	E167	L274	H183	S457	S457		R110	E167	L274	H183	S457	S457
S40	R111	E167	L274	H183	S457	S457		R111	E167	L274	H183	S457	S457
L41	R112	E167	L274	H183	S457	S457		R112	E167	L274	H183	S457	S457
S42	R113	E167	L274	H183	S457	S457		R113	E167	L274	H183	S457	S457
Q43	R114	E167	L274	H183	S457	S457		R114	E167	L274	H183	S457	S457
P44	R115	E167	L274	H183	S457	S457		R115	E167	L274	H183	S457	S457
K45	R116	E167	L274	H183	S457	S457		R116	E167	L274	H183	S457	S457
L51	R117	E167	L274	H183	S457	S457		R117	E167	L274	H183	S457	S457
F52	R118	E167	L274	H183	S457	S457		R118	E167	L274	H183	S457	S457
R53	R119	E167	L274	H183	S457	S457		R119	E167	L274	H183	S457	S457
R54	R120	E167	L274	H183	S457	S457		R120	E167	L274	H183	S457	S457
G55	R121	E167	L274	H183	S457	S457		R121	E167	L274	H183	S457	S457
R55	R122	E167	L274	H183	S457	S457		R122	E167	L274	H183	S457	S457
T56	R123	E167	L274	H183	S457	S457		R123	E167	L274	H183	S457	S457
K60	R124	E167	L274	H183	S457	S457		R124	E167	L274	H183	S457	S457
E66	R125	E167	L274	H183	S457	S457		R125	E167	L274	H183	S457	S457
A67	R126	E167	L274	H183	S457	S457		R126	E167	L274	H183	S457	S457
V68	R127	E167	L274	H183	S457	S457		R127	E167	L274	H183	S457	S457
C69	R128	E167	L274	H183	S457	S457		R128	E167	L274	H183	S457	S457
I70	R129	E167	L274	H183	S457	S457		R129	E167	L274	H183	S457	S457
V71	R130	E167	L274	H183	S457	S457		R130	E167	L274	H183	S457	S457
L72	R131	E167	L274	H183	S457	S457		R131	E167	L274	H183	S457	S457



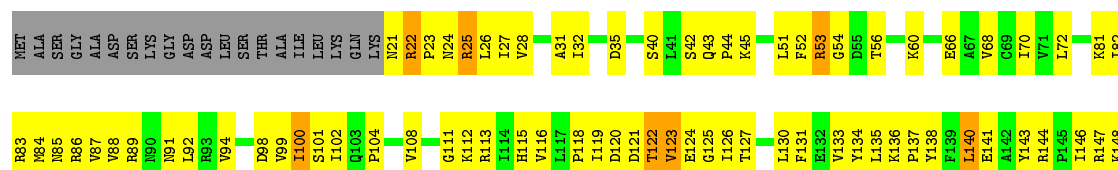
# Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain D: 49% 40% 10%



# Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain E: 49% 40% 10%







[illegible]

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	215000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	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: ADP, OJA

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.45	0/5751	0.65	2/7767 (0.0%)
1	B	0.45	0/5751	0.65	3/7767 (0.0%)
1	C	0.45	0/5751	0.65	2/7767 (0.0%)
1	D	0.45	0/5751	0.65	2/7767 (0.0%)
1	E	0.45	0/5751	0.65	2/7767 (0.0%)
1	F	0.45	0/5751	0.65	3/7767 (0.0%)
All	All	0.45	0/34506	0.65	14/46602 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	F	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	E	140	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	140	LEU	CA-CB-CG	5.42	127.78	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5659	0	5731	470	0
1	B	5659	0	5731	477	0
1	C	5659	0	5731	473	0
1	D	5659	0	5731	473	0
1	E	5659	0	5731	472	0
1	F	5659	0	5731	472	0
2	A	54	0	24	9	0
2	B	54	0	24	10	0
2	C	54	0	24	9	0
2	D	54	0	24	9	0
2	E	54	0	24	9	0
2	F	54	0	24	9	0
3	A	34	0	38	5	0
3	B	34	0	38	4	0
3	C	34	0	38	4	0
3	D	34	0	38	5	0
3	E	34	0	38	3	0
3	F	34	0	38	4	0
4	A	20	0	0	2	0
4	B	20	0	0	2	0
4	C	20	0	0	0	0
4	D	20	0	0	1	0
4	E	20	0	0	1	0
4	F	20	0	0	1	0
All	All	34602	0	34758	2782	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 40.

The worst 5 of 2782 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)
1:F:26:LEU:CD2	1:F:100:ILE:HD12	1.21	1.68
1:B:26:LEU:CD2	1:B:100:ILE:HD12	1.21	1.62
1:E:26:LEU:CD2	1:E:100:ILE:HD12	1.21	1.60
1:C:26:LEU:CD2	1:C:100:ILE:HD12	1.21	1.58
1:D:26:LEU:HD21	1:D:100:ILE:CD1	1.11	1.58

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	Percentiles	
1	A	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	B	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	C	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	D	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	E	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
1	F	719/806 (89%)	671 (93%)	41 (6%)	7 (1%)	19	21
All	All	4314/4836 (89%)	4026 (93%)	246 (6%)	42 (1%)	24	21

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	53	ARG
1	A	123	VAL
1	B	25	ARG
1	B	53	ARG

### 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.

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	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	B	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	C	615/678 (91%)	612 (100%)	3 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	E	615/678 (91%)	612 (100%)	3 (0%)	92	97
1	F	615/678 (91%)	612 (100%)	3 (0%)	92	97
All	All	3690/4068 (91%)	3672 (100%)	18 (0%)	92	97

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	638	ARG
1	D	100	ILE
1	E	638	ARG
1	C	100	ILE
1	C	122	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	568	GLN
1	D	421	GLN
1	F	536	GLN
1	C	616	ASN
1	D	115	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 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$
3	OJA	A	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.68	9 (19%)
2	ADP	A	807	-	24,29,29	0.96	1 (4%)	23,45,45	1.72	1 (4%)
2	ADP	A	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.78	2 (8%)
3	OJA	B	1001	-	37,38,38	0.93	3 (8%)	46,53,53	1.67	10 (21%)
2	ADP	B	807	-	24,29,29	0.96	1 (4%)	23,45,45	1.72	1 (4%)
2	ADP	B	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.77	2 (8%)
3	OJA	C	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.69	8 (17%)
2	ADP	C	807	-	24,29,29	0.95	1 (4%)	23,45,45	1.73	1 (4%)
2	ADP	C	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.79	2 (8%)
3	OJA	D	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.68	9 (19%)
2	ADP	D	807	-	24,29,29	0.96	1 (4%)	23,45,45	1.71	1 (4%)
2	ADP	D	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.78	2 (8%)
3	OJA	E	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.68	10 (21%)
2	ADP	E	807	-	24,29,29	0.96	1 (4%)	23,45,45	1.71	1 (4%)
2	ADP	E	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.79	3 (13%)
3	OJA	F	1001	-	37,38,38	0.94	3 (8%)	46,53,53	1.68	9 (19%)
2	ADP	F	807	-	24,29,29	0.97	1 (4%)	23,45,45	1.71	1 (4%)
2	ADP	F	900	-	24,29,29	0.97	1 (4%)	23,45,45	1.78	2 (8%)

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
3	OJA	A	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	A	807	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	900	-	-	0/12/32/32	0/3/3/3
3	OJA	B	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	B	807	-	-	0/12/32/32	0/3/3/3
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3
3	OJA	C	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	C	807	-	-	0/12/32/32	0/3/3/3
2	ADP	C	900	-	-	0/12/32/32	0/3/3/3
3	OJA	D	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	D	807	-	-	0/12/32/32	0/3/3/3
2	ADP	D	900	-	-	0/12/32/32	0/3/3/3
3	OJA	E	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	E	807	-	-	0/12/32/32	0/3/3/3
2	ADP	E	900	-	-	0/12/32/32	0/3/3/3
3	OJA	F	1001	-	-	0/18/38/38	0/5/5/5
2	ADP	F	807	-	-	0/12/32/32	0/3/3/3
2	ADP	F	900	-	-	0/12/32/32	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1001	OJA	C21-C23	-2.28	1.45	1.48
3	E	1001	OJA	C21-C23	-2.27	1.45	1.48
3	C	1001	OJA	C21-C23	-2.26	1.45	1.48
3	F	1001	OJA	C21-C23	-2.26	1.45	1.48
3	A	1001	OJA	C21-C23	-2.26	1.45	1.48

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	807	ADP	N3-C2-N1	-6.76	123.56	128.87
2	A	807	ADP	N3-C2-N1	-6.72	123.59	128.87
2	F	807	ADP	N3-C2-N1	-6.71	123.60	128.87
2	B	807	ADP	N3-C2-N1	-6.70	123.61	128.87
2	D	807	ADP	N3-C2-N1	-6.70	123.61	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	OJA	5	0
2	A	807	ADP	5	0
2	A	900	ADP	4	0
3	B	1001	OJA	4	0
2	B	807	ADP	5	0
2	B	900	ADP	5	0
3	C	1001	OJA	4	0
2	C	807	ADP	5	0
2	C	900	ADP	4	0
3	D	1001	OJA	5	0
2	D	807	ADP	5	0
2	D	900	ADP	4	0
3	E	1001	OJA	3	0
2	E	807	ADP	5	0
2	E	900	ADP	4	0
3	F	1001	OJA	4	0
2	F	807	ADP	5	0
2	F	900	ADP	4	0

## 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.