



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:16 PM BST

PDB ID : 5FTK
EMDB ID: : EMD-3296
Title : Cryo-EM structure of human p97 bound to ADP
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 : 2.40 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

A user guide is available at

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

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

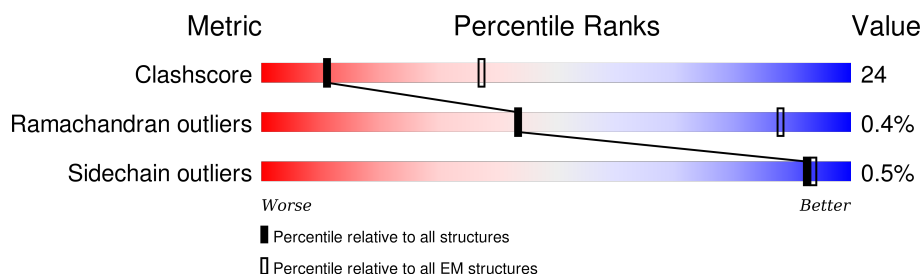
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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 ≥ 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	<div> <div>51%</div> <div>37%</div> <div>• 10%</div> </div>
1	B	806	<div> <div>50%</div> <div>38%</div> <div>• 10%</div> </div>
1	C	806	<div> <div>51%</div> <div>38%</div> <div>• 10%</div> </div>
1	D	806	<div> <div>51%</div> <div>38%</div> <div>• 10%</div> </div>
1	E	806	<div> <div>51%</div> <div>38%</div> <div>• 10%</div> </div>
1	F	806	<div> <div>51%</div> <div>38%</div> <div>• 10%</div> </div>

2 Entry composition [i](#)

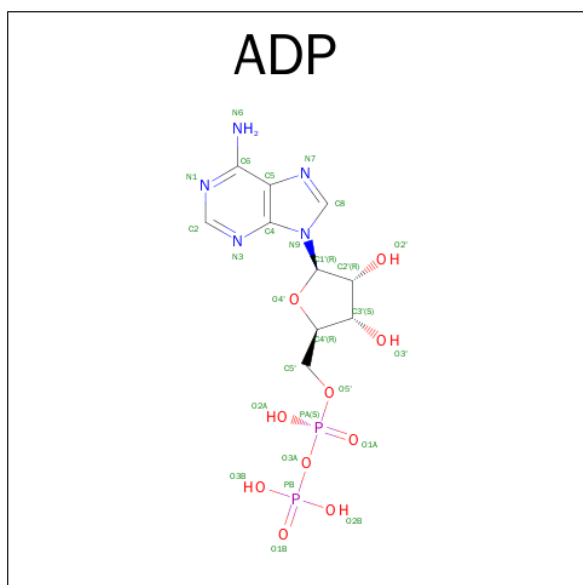
There are 3 unique types of molecules in this entry. The entry contains 34374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_{10}H_{15}N_5O_{10}P_2$).

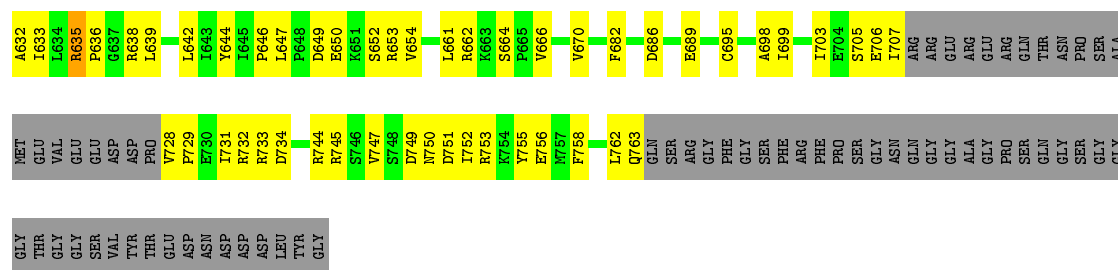


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
2	D	1	Total	C	N	O	P	0
	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

Mol	Chain	Residues	Atoms		AltConf
3	A	16	Total	O	0
			16	16	
3	B	16	Total	O	0
			16	16	
3	C	16	Total	O	0
			16	16	
3	D	16	Total	O	0
			16	16	
3	E	16	Total	O	0
			16	16	
3	F	16	Total	O	0
			16	16	

- Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



ASP	ASP	PRO	V728	P729	E730	I731	R732	R733	D734	M740	R744	R745	S746	V747	S748	D749	N750	D751	I752	R753	K754	V755	E756	R757	F758	L762	O763	G1N	SER	ARG	GLY	PHE	GLY	GLY	SER	PHE	ARG	PHE	PRO	SER	GLY	ASN	GLN	GLY	GLY	ALA	GLY	PRO	SER	GLN	GLY	SER	GLY	GLY	GLY	THR	GLY
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GLY	SER	VAL	TYR	THR	GLU	ASP	ASN	ASP	ASP	ASP	LEU	TYR	GLY
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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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.51	0/5751	0.70	3/7767 (0.0%)
1	B	0.51	0/5751	0.70	3/7767 (0.0%)
1	C	0.51	0/5751	0.70	3/7767 (0.0%)
1	D	0.51	0/5751	0.70	3/7767 (0.0%)
1	E	0.51	0/5751	0.70	3/7767 (0.0%)
1	F	0.51	0/5751	0.70	3/7767 (0.0%)
All	All	0.51	0/34506	0.70	18/46602 (0.0%)

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
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
All	All	0	18

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	THR	N-CA-C	6.01	127.22	111.00
1	F	122	THR	N-CA-C	6.00	127.20	111.00
1	D	122	THR	N-CA-C	6.00	127.19	111.00
1	A	122	THR	N-CA-C	5.99	127.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	THR	N-CA-C	5.99	127.17	111.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ARG	Peptide
1	A	225	ARG	Sidechain
1	A	635	ARG	Sidechain
1	B	210	ARG	Peptide
1	B	225	ARG	Sidechain

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	5659	0	5731	282	0
1	B	5659	0	5731	284	0
1	C	5659	0	5731	281	0
1	D	5659	0	5731	289	0
1	E	5659	0	5731	288	0
1	F	5659	0	5731	286	0
2	A	54	0	24	3	0
2	B	54	0	24	3	0
2	C	54	0	24	3	0
2	D	54	0	24	3	0
2	E	54	0	24	3	0
2	F	54	0	24	3	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
3	E	16	0	0	0	0
3	F	16	0	0	0	0
All	All	34374	0	34530	1630	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 24.

The worst 5 of 1630 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:B:87:VAL:HG12	1:B:198:LEU:HD21	1.44	0.99
1:A:87:VAL:HG12	1:A:198:LEU:HD21	1.44	0.99
1:E:87:VAL:HG12	1:E:198:LEU:HD21	1.44	0.98
1:D:87:VAL:HG12	1:D:198:LEU:HD21	1.44	0.97
1:C:87:VAL:HG12	1:C:198:LEU:HD21	1.44	0.96

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%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	B	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	C	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	D	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	E	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
1	F	719/806 (89%)	672 (94%)	44 (6%)	3 (0%)	39	56
All	All	4314/4836 (89%)	4032 (94%)	264 (6%)	18 (0%)	43	56

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	VAL
1	B	235	VAL
1	C	235	VAL
1	D	235	VAL
1	E	235	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
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	563	PHE
1	D	286	LEU
1	E	563	PHE
1	C	286	LEU
1	C	367	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	443	ASN
1	D	285	ASN
1	F	285	ASN
1	D	50	GLN
1	D	337	GLN

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 ⓘ

12 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	$\# Z > 2$
2	ADP	A	807	-	24,29,29	1.00	1 (4%)	23,45,45	1.90	2 (8%)
2	ADP	A	900	-	24,29,29	0.98	1 (4%)	23,45,45	1.92	4 (17%)
2	ADP	B	807	-	24,29,29	0.99	1 (4%)	23,45,45	1.89	2 (8%)
2	ADP	B	900	-	24,29,29	0.99	1 (4%)	23,45,45	1.93	4 (17%)
2	ADP	C	807	-	24,29,29	1.00	1 (4%)	23,45,45	1.89	2 (8%)
2	ADP	C	900	-	24,29,29	0.98	1 (4%)	23,45,45	1.93	4 (17%)
2	ADP	D	807	-	24,29,29	1.00	1 (4%)	23,45,45	1.91	2 (8%)
2	ADP	D	900	-	24,29,29	0.98	1 (4%)	23,45,45	1.93	4 (17%)
2	ADP	E	807	-	24,29,29	0.99	1 (4%)	23,45,45	1.89	2 (8%)
2	ADP	E	900	-	24,29,29	0.99	1 (4%)	23,45,45	1.92	4 (17%)
2	ADP	F	807	-	24,29,29	1.00	1 (4%)	23,45,45	1.91	2 (8%)
2	ADP	F	900	-	24,29,29	0.99	1 (4%)	23,45,45	1.92	4 (17%)

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
2	ADP	A	807	-	-	0/12/32/32	0/3/3/3
2	ADP	A	900	-	-	0/12/32/32	0/3/3/3
2	ADP	B	807	-	-	0/12/32/32	0/3/3/3
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3
2	ADP	C	807	-	-	0/12/32/32	0/3/3/3
2	ADP	C	900	-	-	0/12/32/32	0/3/3/3
2	ADP	D	807	-	-	0/12/32/32	0/3/3/3
2	ADP	D	900	-	-	0/12/32/32	0/3/3/3
2	ADP	E	807	-	-	0/12/32/32	0/3/3/3
2	ADP	E	900	-	-	0/12/32/32	0/3/3/3
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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	807	ADP	C5-C4	2.21	1.45	1.40
2	E	807	ADP	C5-C4	2.21	1.45	1.40
2	B	807	ADP	C5-C4	2.21	1.45	1.40
2	F	807	ADP	C5-C4	2.22	1.45	1.40
2	A	807	ADP	C5-C4	2.23	1.45	1.40

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	807	ADP	N3-C2-N1	-7.14	123.26	128.87
2	D	807	ADP	N3-C2-N1	-7.14	123.26	128.87
2	A	807	ADP	N3-C2-N1	-7.09	123.30	128.87
2	E	807	ADP	N3-C2-N1	-7.07	123.32	128.87
2	C	807	ADP	N3-C2-N1	-7.07	123.32	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	807	ADP	1	0
2	A	900	ADP	2	0
2	B	807	ADP	1	0
2	B	900	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	807	ADP	1	0
2	C	900	ADP	2	0
2	D	807	ADP	1	0
2	D	900	ADP	2	0
2	E	807	ADP	1	0
2	E	900	ADP	2	0
2	F	807	ADP	1	0
2	F	900	ADP	2	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.