wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:40 PM BST

PDB ID	:	3IZQ
EMDB ID:	:	EMD-1811
Title	:	Structure of the Dom34-Hbs1-GDPNP complex bound to a translating ribosome
Authors	:	Becker, T.; Armache, J.-P.; Jarasch, A.; Anger, A.M.; Villa, E.; Sieber, H.; Abdel Motaal, B.; Mielke, T.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2010-11-30
Resolution	:	9.50 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

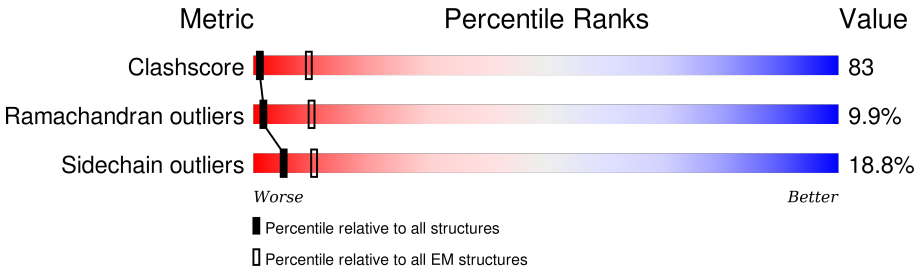
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.50 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 <=5%

Mol	Chain	Length	Quality of chain
1	0	386	38% 35% 19% 7%
2	1	611	27% 38% 13% 6% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7183 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 Protein DOM34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	386	3097	1996	483	603	15	0	0

- Molecule 2 is a protein called Elongation factor 1 alpha-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	516	4086	2589	692	789	16	0	0

There is a discrepancy between the modelled and reference sequences:

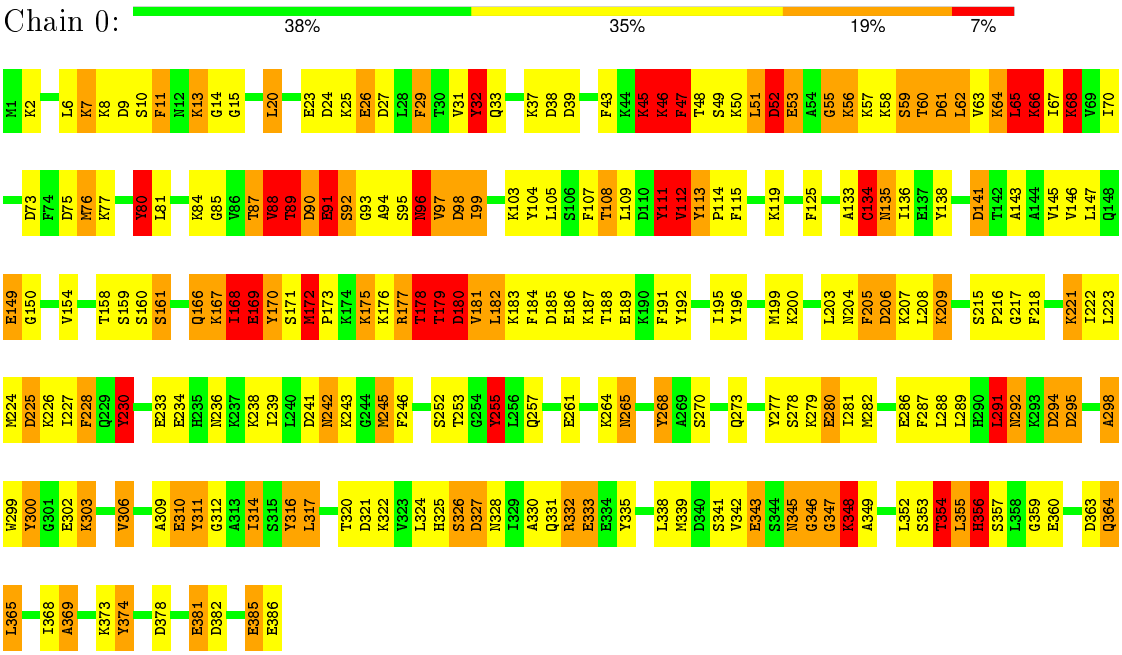
Chain	Residue	Modelled	Actual	Comment	Reference
1	32	GLU	ASP	ENGINEERED MUTATION	UNP P32769

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 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.

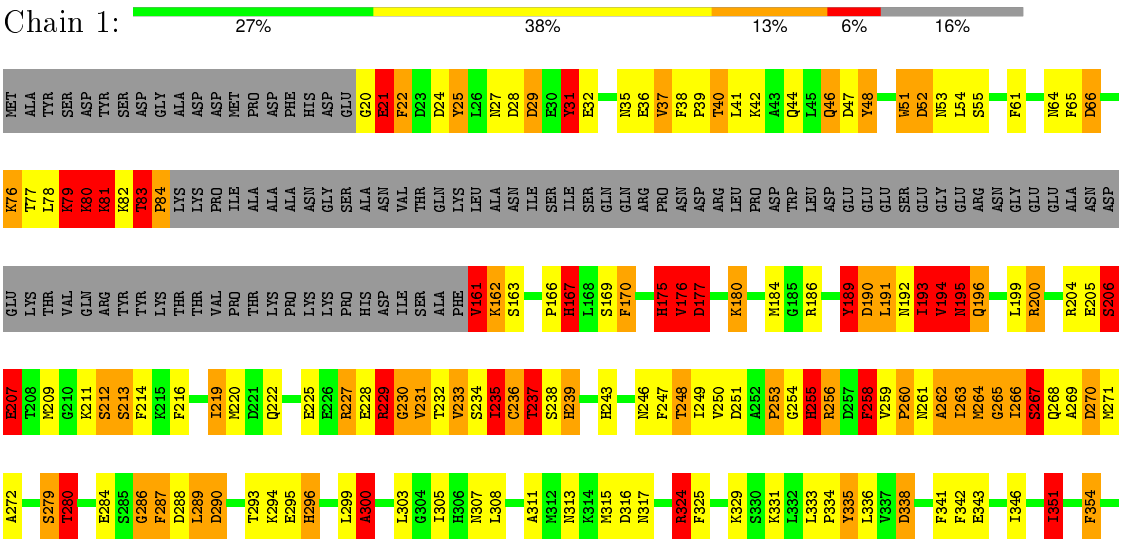
- Molecule 1: Protein DOM34

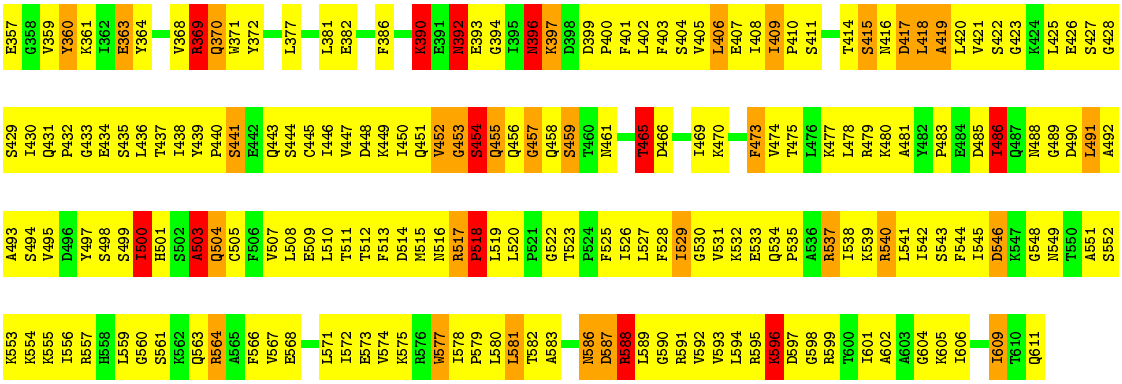
Chain 0:



- Molecule 2: Elongation factor 1 alpha-like protein

Chain 1:




E357 G358 V359 Y360 K361 I362 E363 Y364 V368 R369 Q370 W371 Y372 L377 L381 E382 F386 K390 E391 N392 E393 G394 I395 N396 K397 D398 D399 P400 F401 L402 F403 S404 V405 L406 E407 I408 I409 P410 S411 T414 S415 W416 D417 L418 A419 L420 V421 S422 G423 K424 L425 E426 S427 G428
S429 I430 Q431 P432 G433 E434 S435 L436 T437 I438 Y439 P440 S441 E442 Q443 S444 C445 I446 V447 D448 K449 I450 Q451 V452 G453 S454 Q455 Q456 G457 Q458 S459 T460 N461 T465 D466 I469 K470 F473 V474 T475 L476 K477 L478 R479 K480 A481 Y482 P483 E484 D485 I486 Q487 N488 G489 D490 L491 A492
A493 S494 V495 D496 Y497 S498 S499 I500 H501 S502 A503 Q504 C505 F506 V507 L508 E509 L510 T511 T512 F513 D514 M515 N516 R517 P518 L519 L520 P521 G522 T523 P524 F525 I526 L527 F528 I529 G530 V531 K532 E533 Q534 P535 A536 R537 I538 K539 R540 L541 I542 S543 F544 I545 D546 K547 G548 N549 T550 A551 S552
K553 K554 K555 I556 R557 H558 L559 G560 S561 K562 Q563 R564 A565 F566 V567 E568 L571 I572 E573 V574 K575 R576 W577 I578 P579 L580 L581 T582 A583 N586 D587 R588 L589 G590 R591 V592 V593 L594 R595 K596 D597 G598 R599 T600 I601 A602 A603 G604 K605 I606 I609 T610 Q611

4 Experimental information (i)

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	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2500	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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	0	1.63	35/3149 (1.1%)	2.13	143/4230 (3.4%)
2	1	1.44	15/4162 (0.4%)	2.06	171/5618 (3.0%)
All	All	1.52	50/7311 (0.7%)	2.09	314/9848 (3.2%)

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	0	6	22
2	1	4	26
All	All	10	48

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	168	ILE	CG1-CD1	17.39	2.70	1.50
1	0	99	ILE	CG1-CD1	12.90	2.39	1.50
1	0	91	GLU	CG-CD	9.53	1.66	1.51
2	1	235	ILE	N-CA	-8.54	1.29	1.46
1	0	65	LEU	CA-CB	8.46	1.73	1.53

The worst 5 of 314 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	65	LEU	CB-CG-CD2	18.11	141.79	111.00
1	0	11	PHE	CB-CG-CD1	17.04	132.73	120.80
2	1	372	TYR	CB-CG-CD2	-15.99	111.41	121.00
1	0	11	PHE	CB-CG-CD2	-14.97	110.32	120.80
1	0	11	PHE	N-CA-CB	13.84	135.51	110.60

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	11	PHE	CA
1	0	56	LYS	CA
1	0	65	LEU	CA
1	0	90	ASP	CA
1	0	91	GLU	CA

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	14	GLY	Peptide
1	0	32	TYR	Sidechain
1	0	47	PHE	Mainchain
1	0	48	THR	Peptide
1	0	51	LEU	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	3097	0	3156	613	0
2	1	4086	0	4068	688	0
All	All	7183	0	7224	1200	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 83.

The worst 5 of 1200 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)
1:0:170:TYR:CD1	1:0:187:LYS:HE3	1.35	1.60
1:0:45:LYS:HE2	1:0:47:PHE:CD2	1.35	1.60
1:0:170:TYR:CG	1:0:187:LYS:HE3	1.33	1.60
1:0:173:PRO:CB	1:0:184:PHE:CE2	1.76	1.59
1:0:314:ILE:HD12	1:0:342:VAL:CG1	1.34	1.58

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 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	0	384/386 (100%)	302 (79%)	46 (12%)	36 (9%)	1 16
2	1	512/611 (84%)	410 (80%)	49 (10%)	53 (10%)	1 12
All	All	896/997 (90%)	712 (80%)	95 (11%)	89 (10%)	2 14

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	15	GLY
1	0	46	LYS
1	0	51	LEU
1	0	52	ASP
1	0	56	LYS

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	0	348/348 (100%)	280 (80%)	68 (20%)	2 12
2	1	456/538 (85%)	373 (82%)	83 (18%)	2 15
All	All	804/886 (91%)	653 (81%)	151 (19%)	5 13

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	21	GLU

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Mol	Chain	Res	Type
2	1	177	ASP
2	1	483	PRO
2	1	31	TYR
2	1	80	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	1	261	ASN
2	1	396	ASN
2	1	504	GLN
2	1	195	ASN
2	1	488	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.