wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:55 PM BST

PDB ID	:	3ZW6
EMDB ID:	:	EMD-1940
Title	:	MODEL OF HEXAMERIC AAA DOMAIN ARRANGEMENT OF GREEN-TYPE RUBISCO ACTIVASE FROM TOBACCO.
Authors	:	Stotz, M.; Mueller-Cajar, O.; Ciniawsky, S.; Wendler, P.; Hartl, F.U.; Bracher, A.; Hayer-Hartl, M.
Deposited on	:	2011-07-28
Resolution	:	20.00 Å(reported)
Based on PDB ID	:	3T15

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

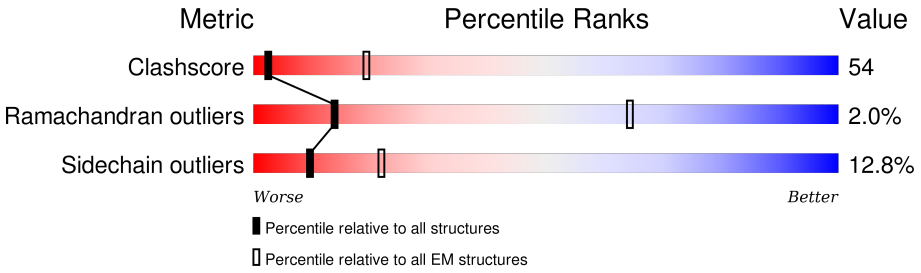
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 20.00 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	A	293	39% 43% 7% 10%
1	B	293	39% 43% 8% 10%
1	C	293	40% 43% 7% 10%
1	D	293	40% 43% 7% 10%
1	E	293	39% 43% 7% 10%
1	F	293	39% 43% 7% 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12492 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 RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC.

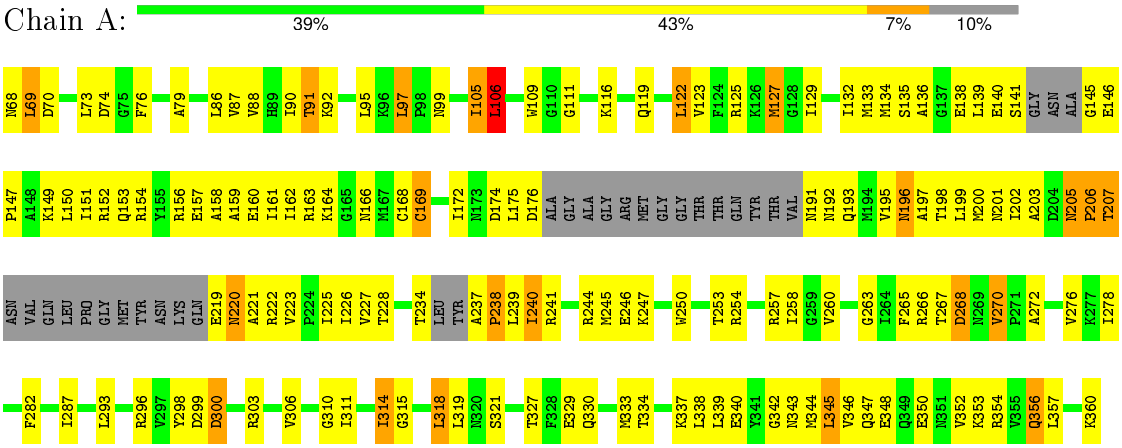
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	B	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	C	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	D	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	E	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	F	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		

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.

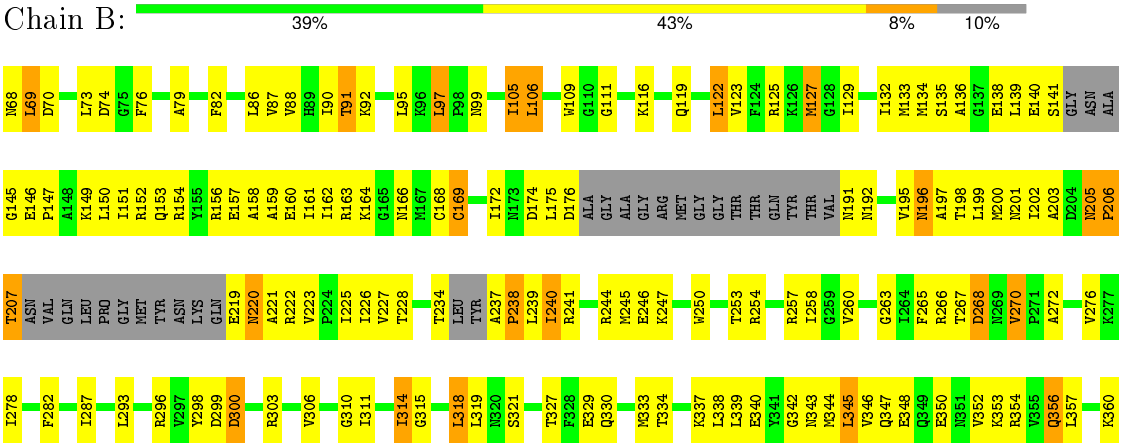
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

Chain A:



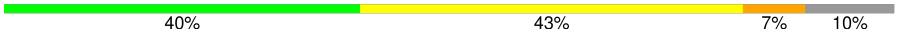
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

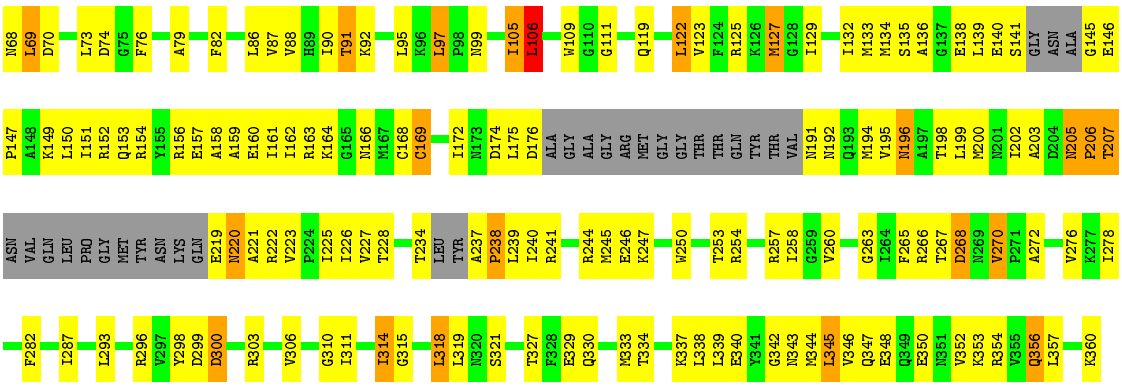
Chain B:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

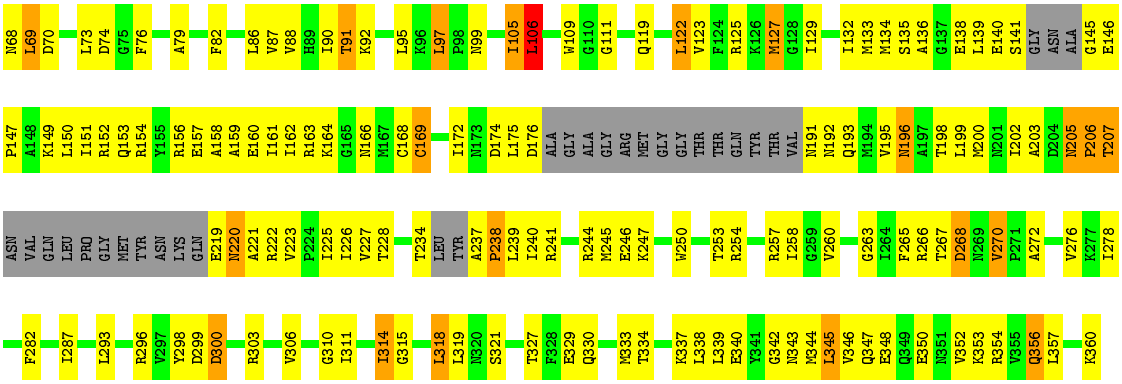
Chain C:





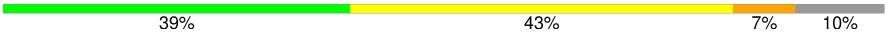
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

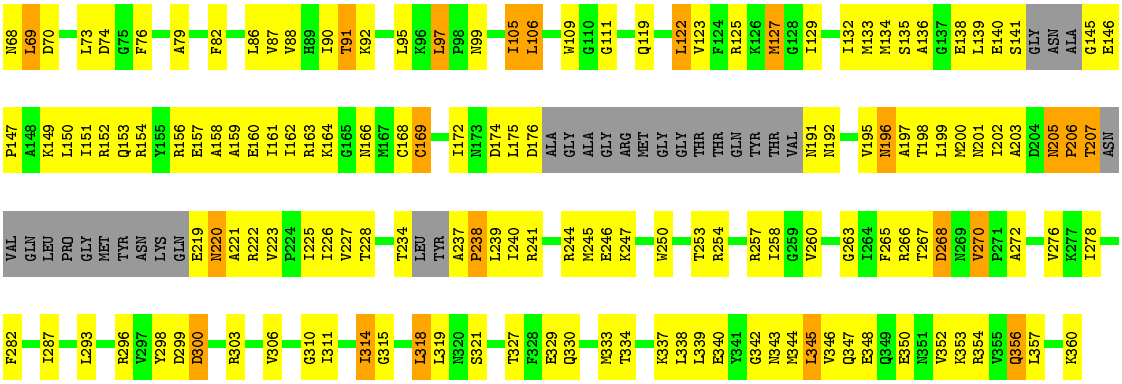
Chain D:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

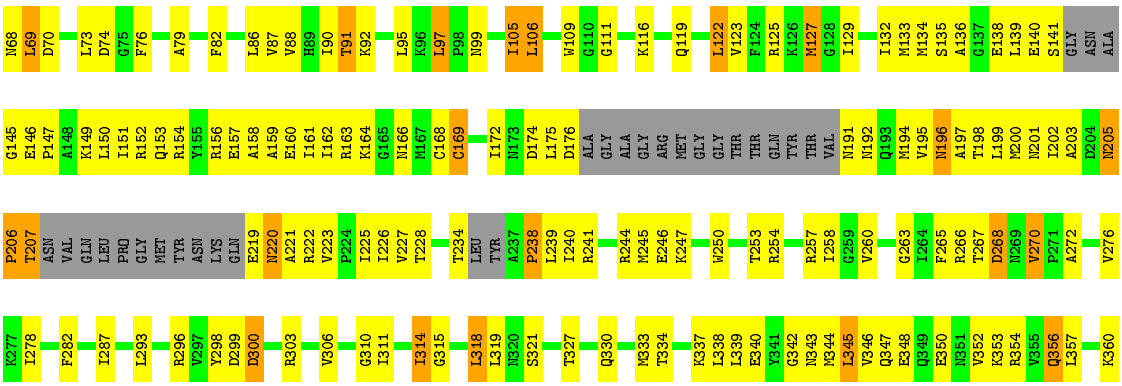
Chain E:





• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

Chain F:


N68 L69 D70 L73 D74 G75 F76 A79 F82 L86 V87 V88 H89 I90 T91 K92 L95 K96 L97 P98 N99 I105 L106 W109 G110 G111 K116 Q119 L122 V123 F124 R125 K126 M127 G128 I129 I132 M133 M134 S135 A136 G137 E138 L139 E140 S141 GLY ASN ALA
G145 E146 P147 A148 K149 L150 I151 R152 Q153 R154 Y155 R156 E157 A158 A159 E160 I161 I162 R163 K164 G165 N166 M167 C168 C169 I172 N173 D174 L175 D176 ALA GLY ALA GLY ARG MET GLY GLY THR THR GLN TYR THR VAL N191 N192 Q193 N194 V195 N196 A197 T198 L199 M200 N201 I202 A203 D204 M205
P206 T207 ASN VAL GLN LEU PRO GLY MET TYR ASN LYS GLN E219 N220 A221 R222 V223 P224 I225 I226 V227 T228 T234 LEU TYR A237 P238 L239 I240 R241 R244 M245 E246 K247 W250 T253 R254 R257 I258 G259 V260 G263 I264 F265 R266 T267 D268 N269 V270 P271 A272 V276
M277 I278 F282 I287 L293 R296 Y297 Y298 D299 D300 R303 V306 G310 I311 I314 G315 I318 L319 N320 S321 T327 Q330 M333 T334 K337 L338 L339 E340 Y341 G342 N343 M344 L345 V346 Q347 E348 Q349 E350 N351 V352 K353 R354 Y355 Q356 L357 K360

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	PHASE FLIPPING, EACH PARTICLE	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	470	Depositor
Maximum defocus (nm)	950	Depositor
Magnification	Not provided	Depositor
Image detector	EAGLE 2K CCD	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	A	0.68	4/2116 (0.2%)	0.68	1/2847 (0.0%)
1	B	0.67	4/2116 (0.2%)	0.68	0/2847
1	C	0.68	4/2116 (0.2%)	0.68	1/2847 (0.0%)
1	D	0.68	4/2116 (0.2%)	0.68	1/2847 (0.0%)
1	E	0.67	4/2116 (0.2%)	0.68	0/2847
1	F	0.67	4/2116 (0.2%)	0.68	0/2847
All	All	0.68	24/12696 (0.2%)	0.68	3/17082 (0.0%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	207	THR	C-O	13.25	1.48	1.23
1	C	207	THR	C-O	13.21	1.48	1.23
1	B	207	THR	C-O	13.19	1.48	1.23
1	A	207	THR	C-O	13.16	1.48	1.23
1	E	207	THR	C-O	13.16	1.48	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	106	LEU	CA-CB-CG	5.06	126.93	115.30
1	C	106	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	106	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2082	0	2097	233	0
1	B	2082	0	2097	231	0
1	C	2082	0	2097	236	0
1	D	2082	0	2097	231	0
1	E	2082	0	2097	226	0
1	F	2082	0	2097	234	0
All	All	12492	0	12582	1360	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 54.

The worst 5 of 1360 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:160:GLU:HA	1:B:163:ARG:HG2	1.28	1.14
1:E:160:GLU:HA	1:E:163:ARG:HG2	1.28	1.13
1:A:109:TRP:HE1	1:A:247:LYS:HG2	1.09	1.13
1:F:160:GLU:HA	1:F:163:ARG:HG2	1.28	1.11
1:F:160:GLU:HA	1:F:163:ARG:CG	1.81	1.11

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	251/293 (86%)	216 (86%)	30 (12%)	5 (2%)	9 51
1	B	251/293 (86%)	216 (86%)	30 (12%)	5 (2%)	9 51
1	C	251/293 (86%)	218 (87%)	28 (11%)	5 (2%)	9 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	251/293 (86%)	216 (86%)	30 (12%)	5 (2%)	9 51
1	E	251/293 (86%)	217 (86%)	29 (12%)	5 (2%)	9 51
1	F	251/293 (86%)	216 (86%)	30 (12%)	5 (2%)	9 51
All	All	1506/1758 (86%)	1299 (86%)	177 (12%)	30 (2%)	14 51

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	PRO
1	A	327	THR
1	B	206	PRO
1	B	327	THR
1	C	206	PRO

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	227/248 (92%)	198 (87%)	29 (13%)	5 29
1	B	227/248 (92%)	198 (87%)	29 (13%)	5 29
1	C	227/248 (92%)	198 (87%)	29 (13%)	5 29
1	D	227/248 (92%)	198 (87%)	29 (13%)	5 29
1	E	227/248 (92%)	198 (87%)	29 (13%)	5 29
1	F	227/248 (92%)	198 (87%)	29 (13%)	5 29
All	All	1362/1488 (92%)	1188 (87%)	174 (13%)	10 29

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	296	ARG
1	D	176	ASP
1	F	228	THR
1	C	314	ILE

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Mol	Chain	Res	Type
1	D	70	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	205	ASN
1	D	166	ASN
1	F	196	ASN
1	C	269	ASN
1	D	93	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.