wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:42 PM BST

PDB ID	:	3J1O
EMDB ID:	:	EMD-5407
Title	:	Cryo-EM map of a yeast minimal preinitiation complex interacting with the Mediator Head module
Authors	:	Asturias, F.J.; Imasaki, T.
Deposited on	:	2012-03-29
Resolution	:	16.00 Å(reported)
Based on PDB ID	:	3RJ1

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

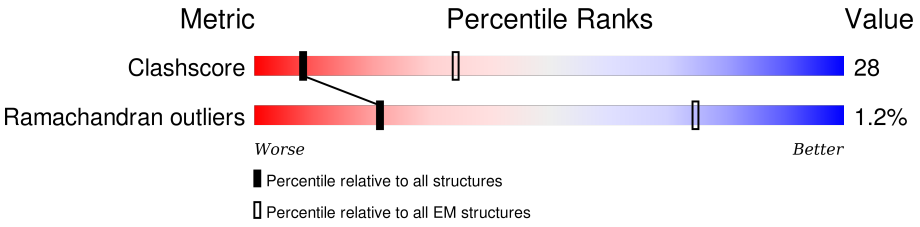
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 16.00 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

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	H	131	57% 15% 28%
2	I	484	52% 13% • 34%
3	J	223	48% 21% • 29%
4	K	121	46% 26% 27%
5	L	275	59% 25% 16%
6	M	210	81% 16% •
7	N	25	84% 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5560 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 Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	H	94	Total	C	N	O	0	0
			468	280	94	94		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	16	GLY	THR	ENGINEERED MUTATION	UNP A0A0D3YMY9
H	17	SER	MET	ENGINEERED MUTATION	UNP A0A0D3YMY9

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	318	Total	C	N	O	0	0
			1583	947	318	318		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	159	Total	C	N	O	0	0
			791	473	159	159		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	88	Total	C	N	O	0	0
			440	264	88	88		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	231	Total	C	N	O	0	0
			1141	679	231	231		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	205	Total	C	N	O	0	0
			1012	602	205	205		

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 6.

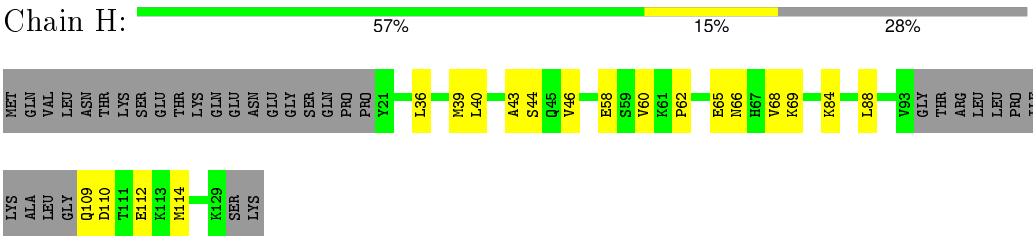
Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	25	Total	C	N	O	0	0
			125	75	25	25		

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.

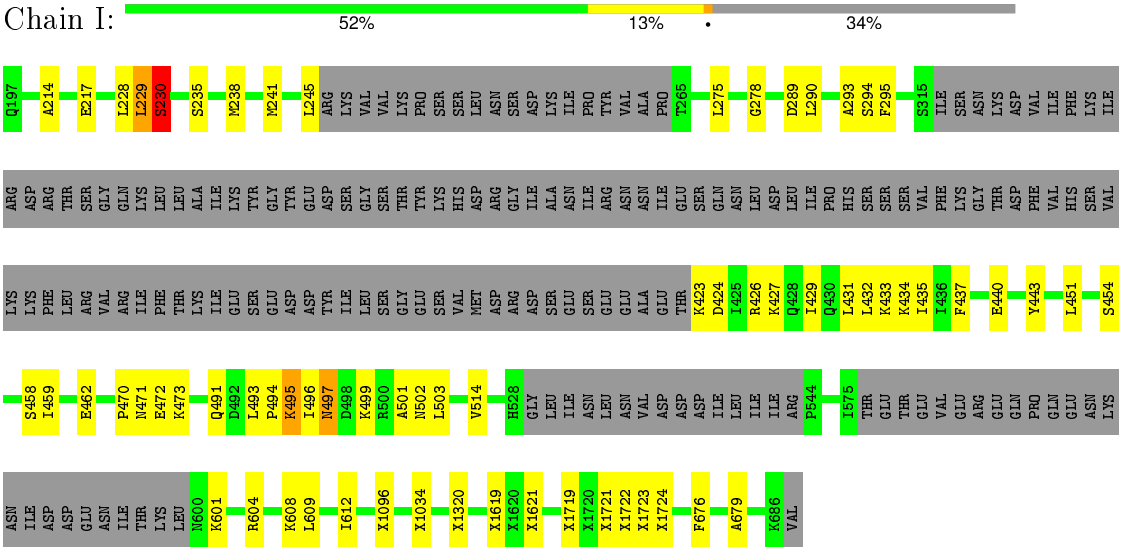
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11

Chain H:



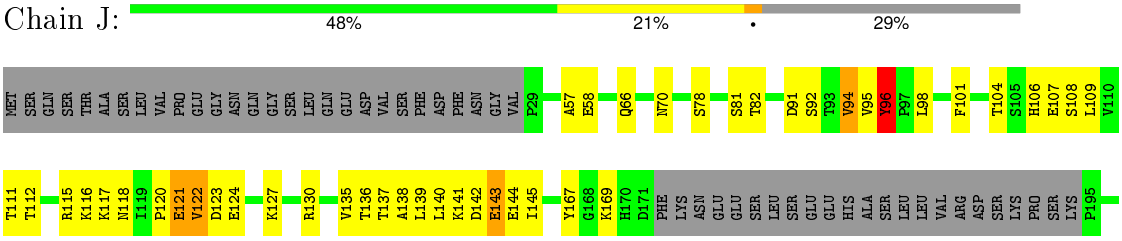
- Molecule 2: Mediator of RNA polymerase II transcription subunit 17

Chain I:



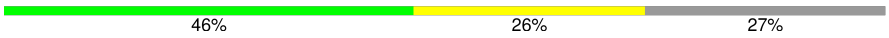
- Molecule 3: Mediator of RNA polymerase II transcription subunit 8

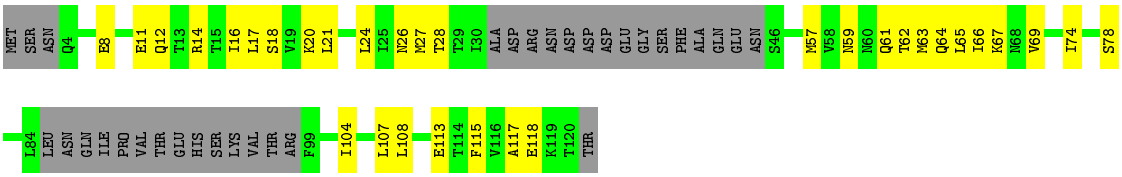
Chain J:



• Molecule 4: Mediator of RNA polymerase II transcription subunit 22

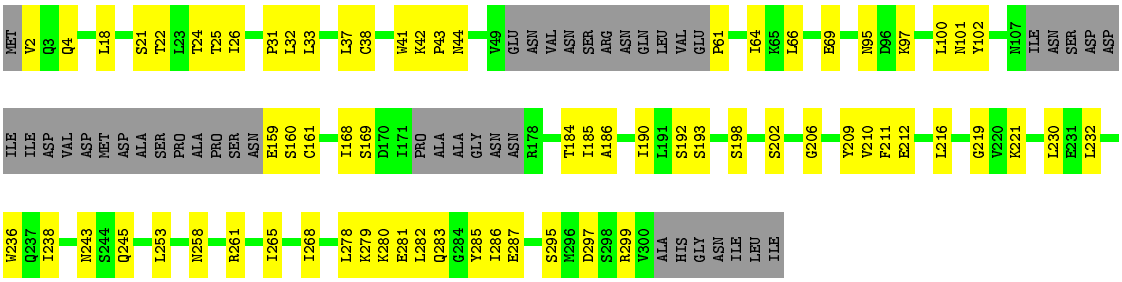
Chain K:





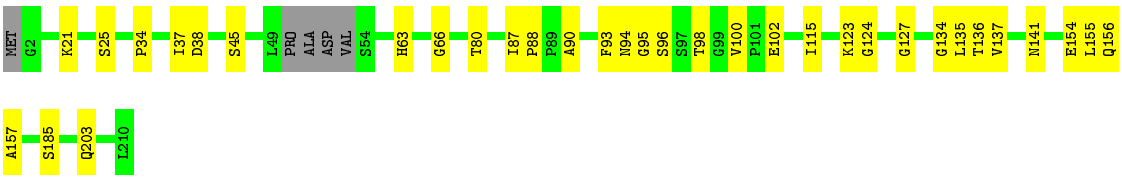
• Molecule 5: Mediator of RNA polymerase II transcription subunit 18

Chain L:



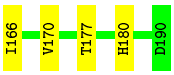
• Molecule 6: Mediator of RNA polymerase II transcription subunit 20

Chain M:



• Molecule 7: Mediator of RNA polymerase II transcription subunit 6

Chain N:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	51000	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each CCD frame	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	50000	Depositor
Image detector	Tietz F415 4kx4k CCD camera	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	H	0.35	0/466	0.57	0/648
2	I	0.38	0/1354	0.70	1/1883 (0.1%)
3	J	0.41	0/789	0.75	2/1099 (0.2%)
4	K	0.40	0/437	0.65	0/607
5	L	0.35	0/1137	0.62	0/1577
6	M	0.35	0/1010	0.65	0/1403
7	N	0.37	0/124	0.64	0/172
All	All	0.37	0/5317	0.67	3/7389 (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
2	I	0	2
3	J	0	4
5	L	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	98	LEU	C-N-CA	6.53	149.41	122.00
2	I	495	LYS	N-CA-C	-5.89	95.10	111.00
3	J	121	GLU	N-CA-C	-5.72	95.55	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	1722	UNK	Peptide
2	I	230	SER	Mainchain
3	J	101	PHE	Peptide
3	J	104	THR	Peptide
3	J	96	TYR	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	H	468	0	192	11	0
2	I	1583	0	625	82	0
3	J	791	0	333	52	0
4	K	440	0	188	22	0
5	L	1141	0	477	88	0
6	M	1012	0	469	18	0
7	N	125	0	49	4	0
All	All	5560	0	2333	224	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 28.

The worst 5 of 224 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:I:432:LEU:N	5:L:22:THR:CB	1.79	1.44
2:I:427:LYS:CB	5:L:285:TYR:CB	1.96	1.40
2:I:433:LYS:CB	5:L:22:THR:C	1.99	1.29
2:I:433:LYS:HA	5:L:25:THR:CB	1.69	1.23
2:I:423:LYS:HA	5:L:281:GLU:C	1.59	1.21

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	H	90/131 (69%)	83 (92%)	7 (8%)	0	100 100
2	I	261/484 (54%)	239 (92%)	17 (6%)	5 (2%)	10 52
3	J	155/223 (70%)	135 (87%)	14 (9%)	6 (4%)	4 36
4	K	82/121 (68%)	69 (84%)	13 (16%)	0	100 100
5	L	223/275 (81%)	193 (86%)	30 (14%)	0	100 100
6	M	201/210 (96%)	184 (92%)	16 (8%)	1 (0%)	34 77
7	N	23/25 (92%)	23 (100%)	0	0	100 100
All	All	1035/1469 (70%)	926 (90%)	97 (9%)	12 (1%)	21 61

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	230	SER
3	J	94	VAL
3	J	144	GLU
2	I	497	ASN
3	J	95	VAL

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.