wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:59 PM BST

PDB ID	:	3JA8
EMDB ID:	:	EMD-6338
Title	:	Cryo-EM structure of the MCM2-7 double hexamer
Authors	:	Li, N.; Zhai, Y.; Zhang, Y.; Li, W.; Yang, M.; Lei, J.; Tye, B.K.; Gao, N.
Deposited on	:	2015-05-09
Resolution	:	3.80 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

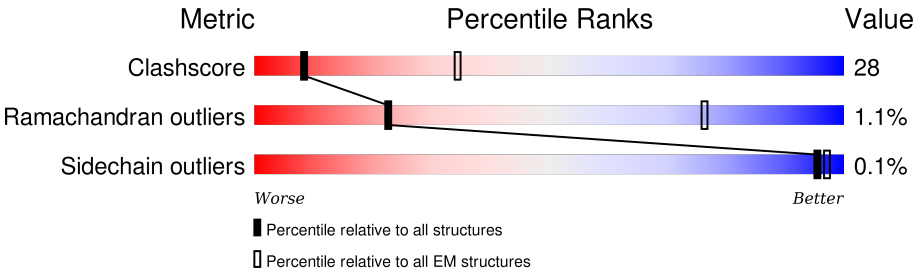
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	2	868	37% 32% • 31%
2	3	971	31% 30% • 38%
3	4	933	34% 34% • 31%
4	5	775	45% 36% 18%
5	6	1017	32% 28% • 39%
6	7	845	42% 38% • 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ADP	6	2001	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29838 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 Minichromosome Maintenance 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	603	4714	2974	842	881	17	0	0

- Molecule 2 is a protein called Minichromosome Maintenance 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	605	4745	2990	846	896	13	0	0

- Molecule 3 is a protein called Minichromosome Maintenance 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	640	5081	3194	879	981	27	0	0

- Molecule 4 is a protein called Minichromosome Maintenance 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	633	4962	3112	855	971	24	0	0

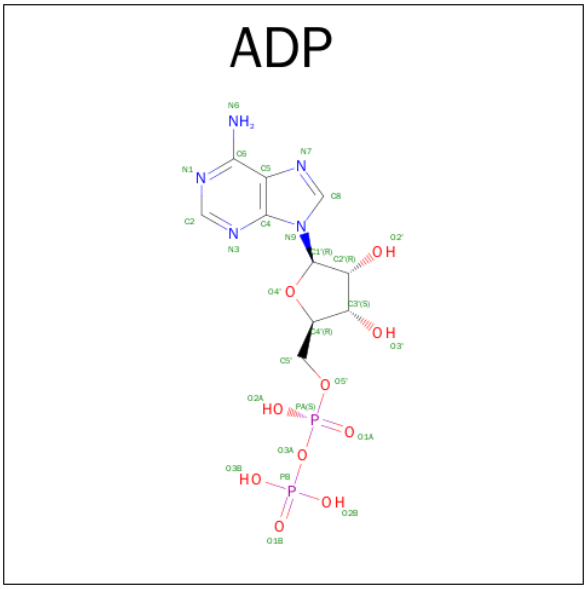
- Molecule 5 is a protein called Minichromosome Maintenance 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	616	4742	2985	841	896	20	0	0

- Molecule 6 is a protein called Minichromosome Maintenance 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	689	5432	3419	940	1042	31	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



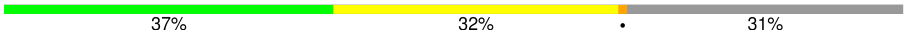
Mol	Chain	Residues	Atoms					AltConf
7	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

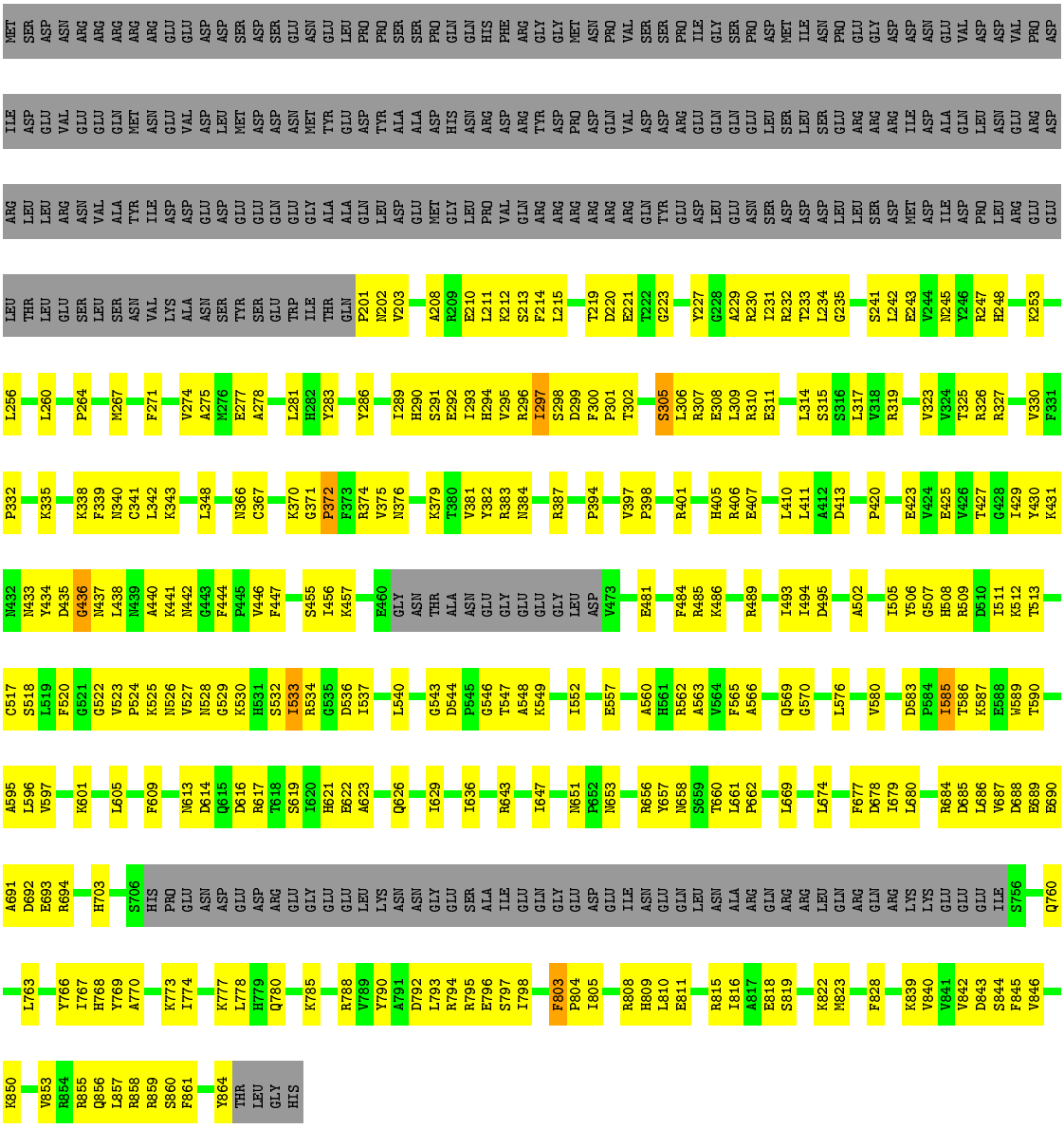
3 Residue-property plots (i)

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: Minichromosome Maintenance 2

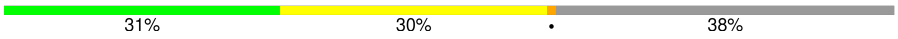
Chain 2:

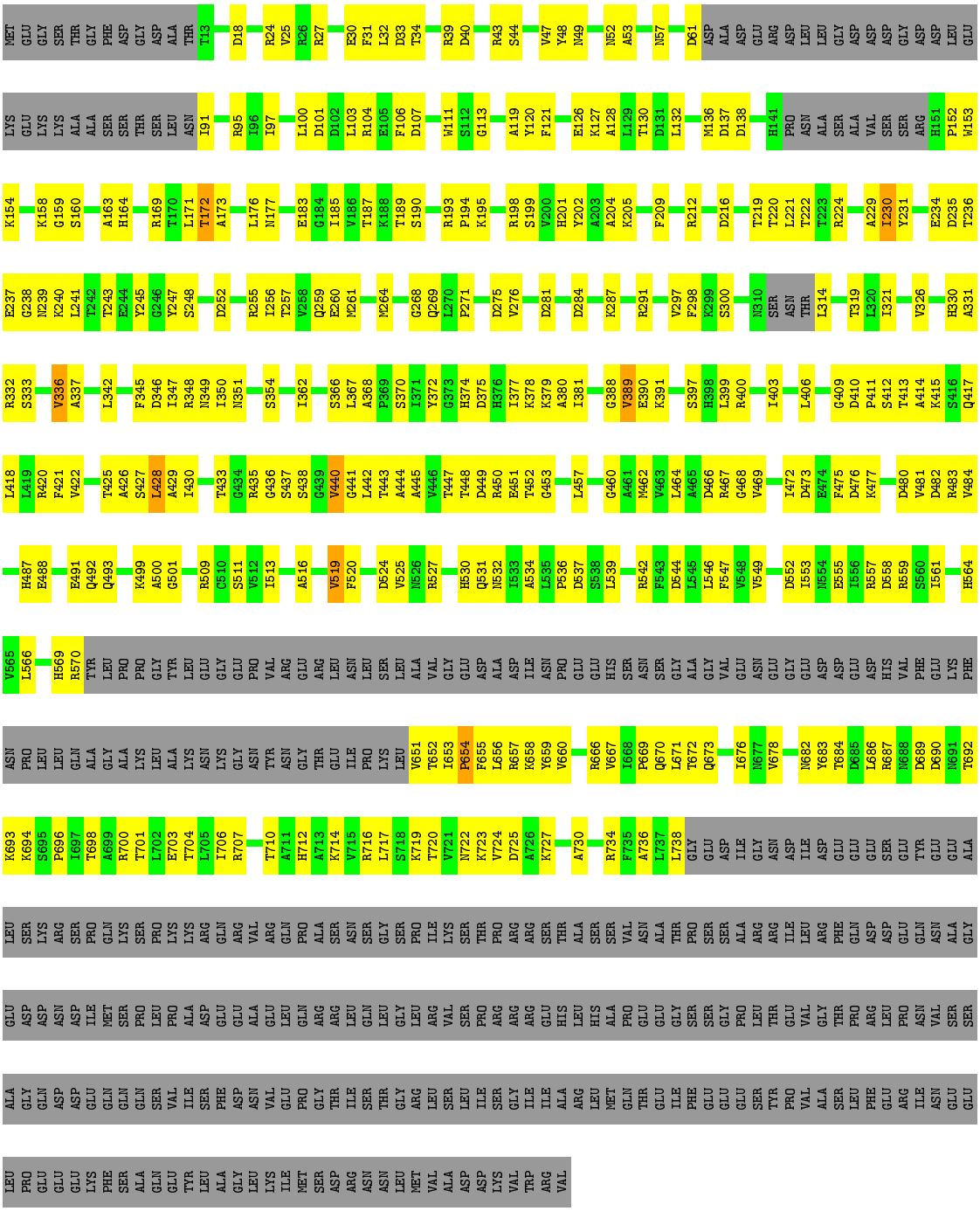




- Molecule 2: Minichromosome Maintenance 3

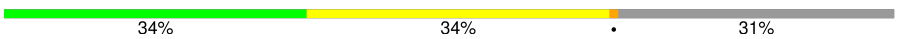
Chain 3:

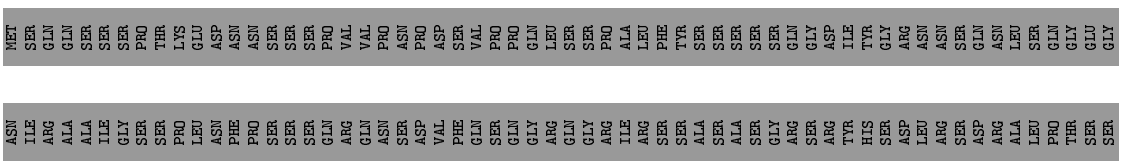


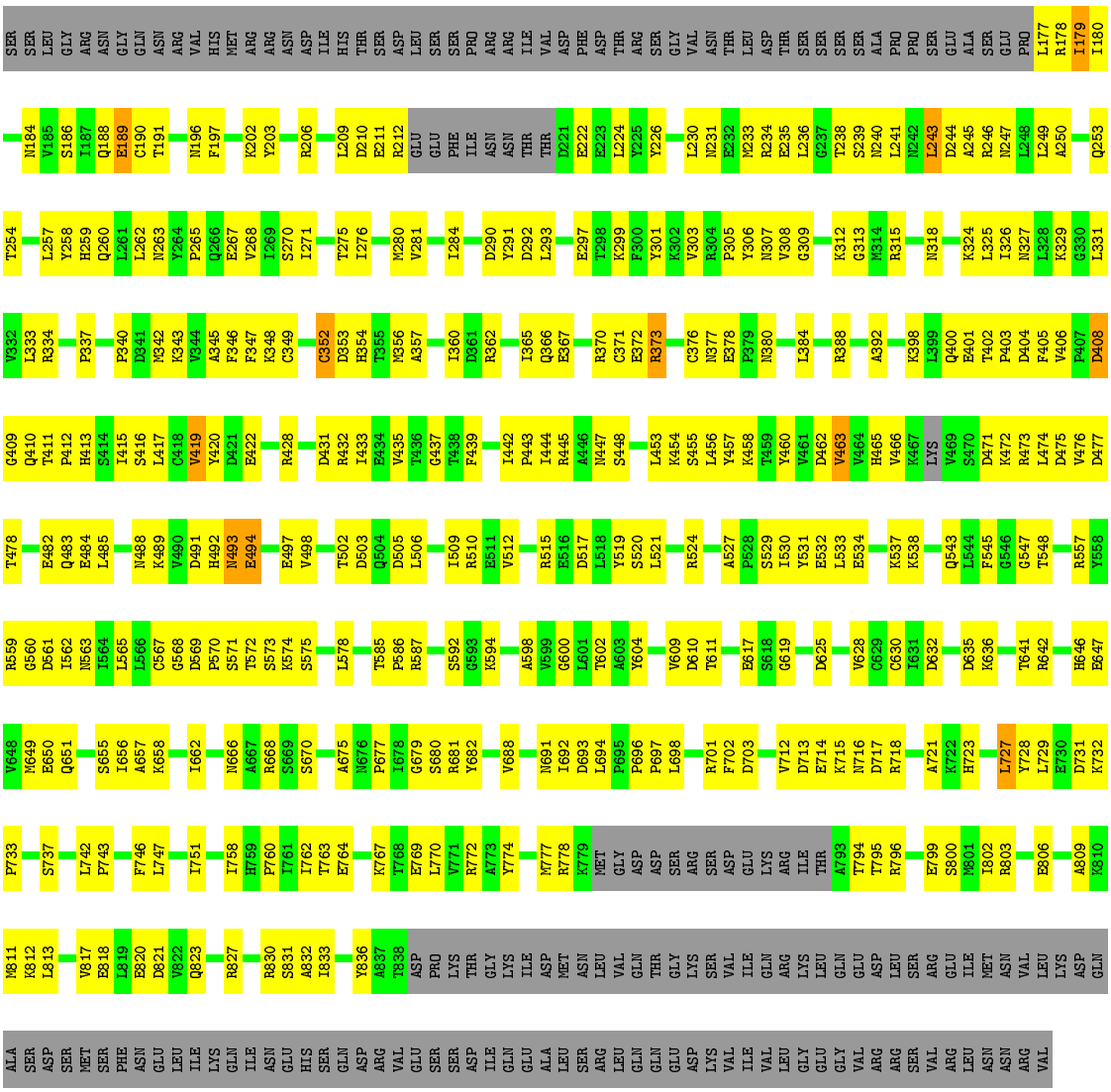


• Molecule 3: Minichromosome Maintenance 4

Chain 4:

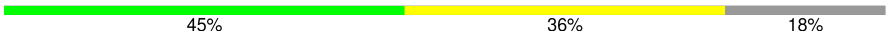


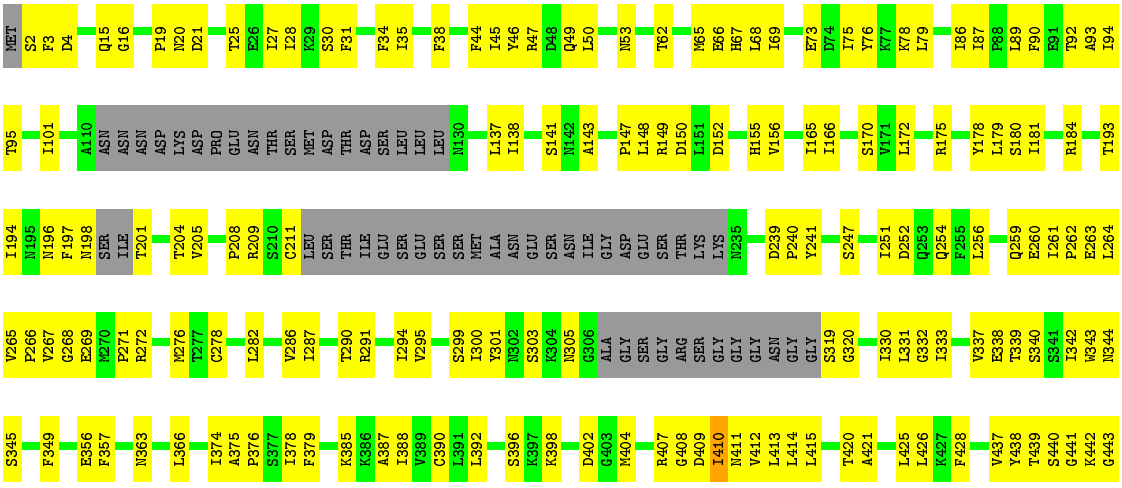


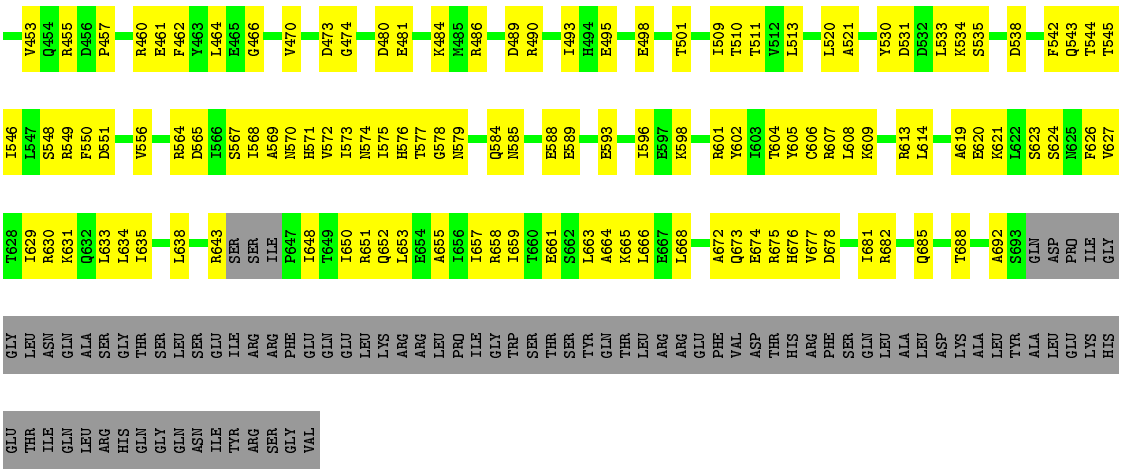


• Molecule 4: Minichromosome Maintenance 5

Chain 5:

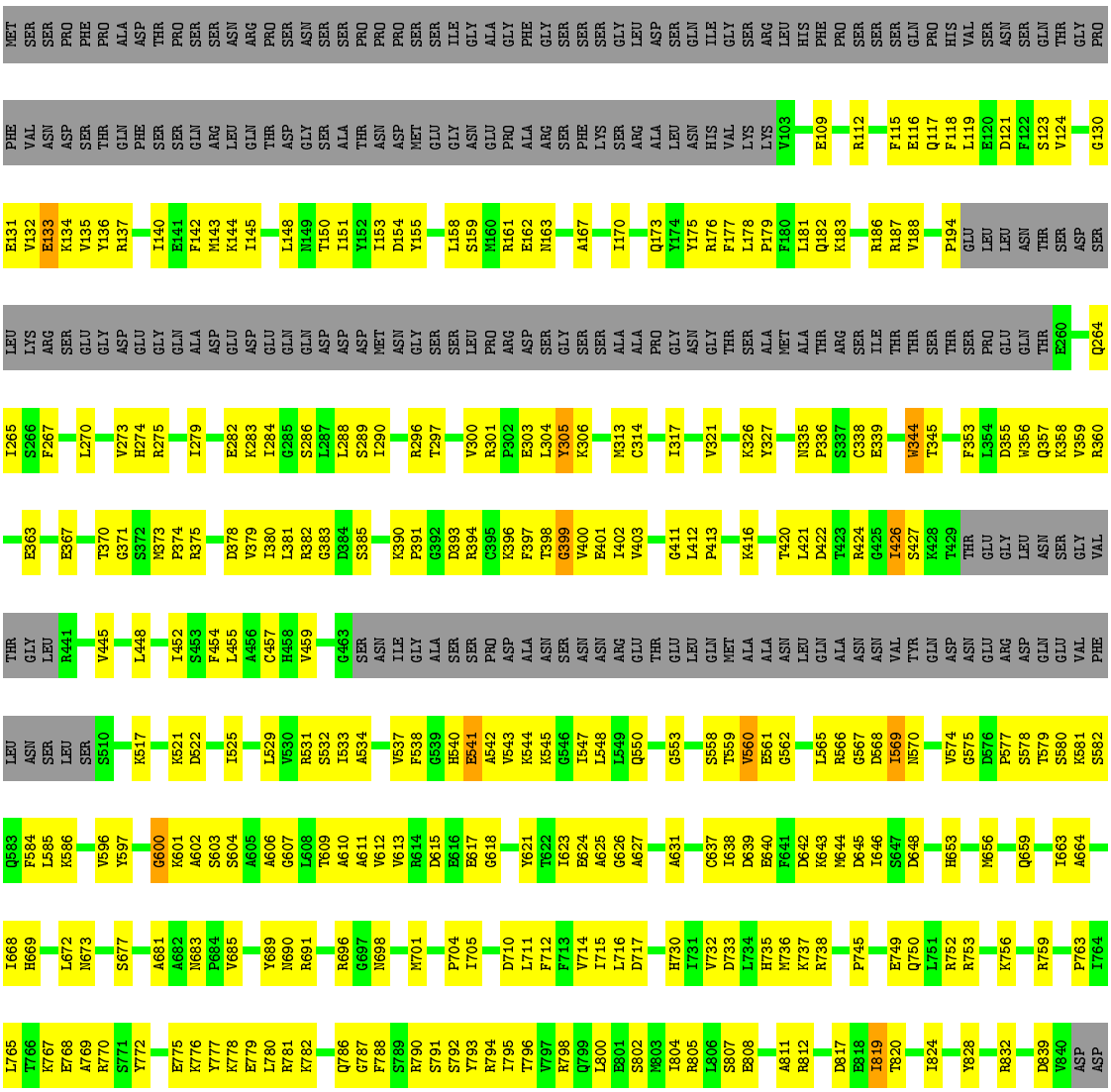


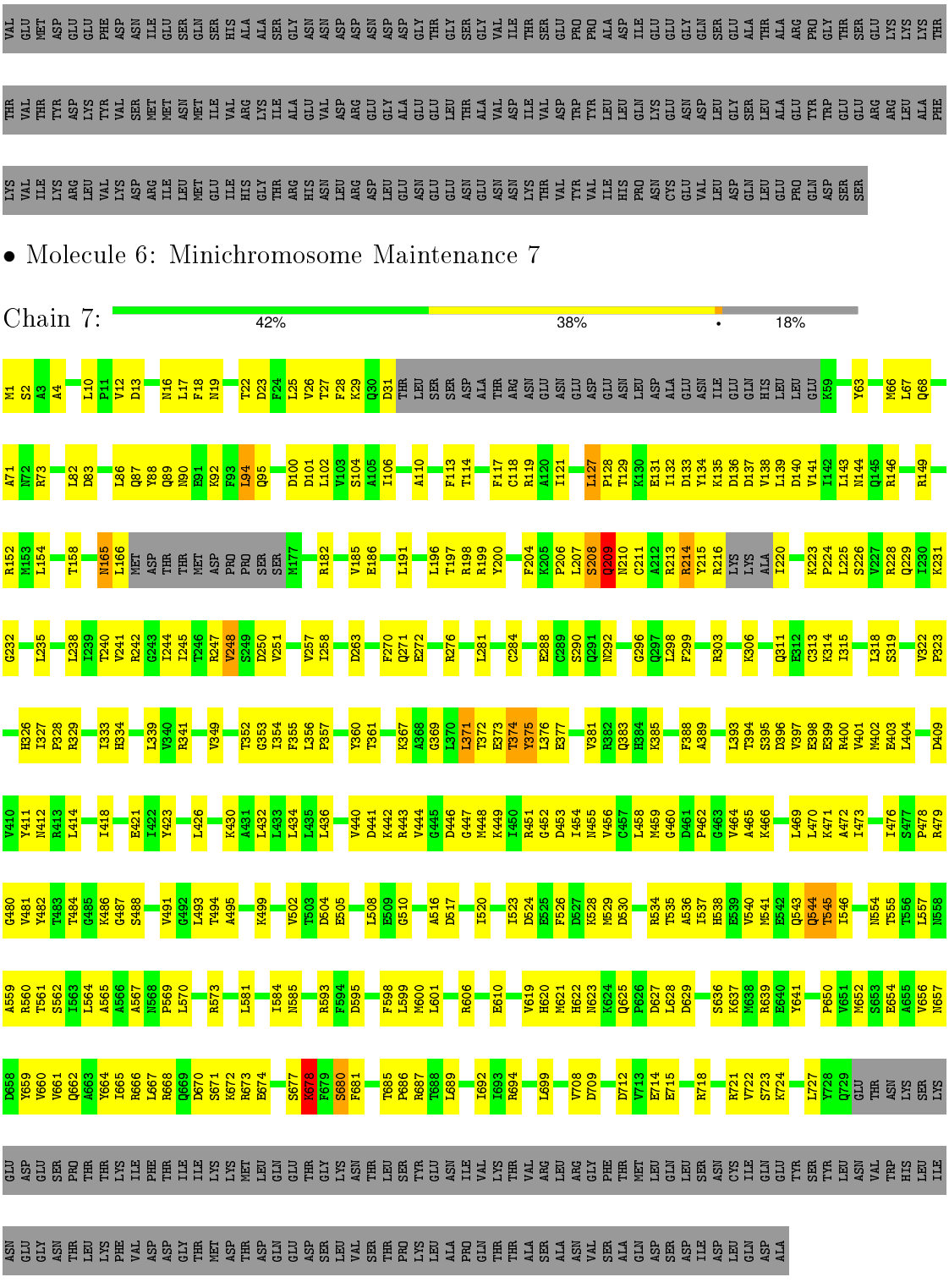




• Molecule 5: Minichromosome Maintenance 6

Chain 6:





• Molecule 6: Minichromosome Maintenance 7

Chain 7: 42% 38% • 18%

4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	85365	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	22	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 (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	2	0.41	0/4794	0.64	2/6479 (0.0%)
2	3	0.48	0/4827	0.67	1/6545 (0.0%)
3	4	0.45	0/5154	0.67	4/6967 (0.1%)
4	5	0.46	0/5032	0.62	0/6799
5	6	0.40	0/4812	0.65	1/6497 (0.0%)
6	7	0.47	0/5514	0.65	3/7450 (0.0%)
All	All	0.45	0/30133	0.65	11/40737 (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	2	0	4
2	3	0	2
3	4	0	3
5	6	0	5
6	7	0	5
All	All	0	19

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3	654	PRO	CA-N-CD	-8.68	99.35	111.50
5	6	399	GLY	N-CA-C	6.81	130.12	113.10
6	7	127	LEU	CA-CB-CG	6.30	129.79	115.30
6	7	209	GLN	N-CA-C	-6.27	94.06	111.00
3	4	243	LEU	CA-CB-CG	5.94	128.96	115.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	367	CYS	Peptide
1	2	372	PRO	Peptide
1	2	436	GLY	Peptide
1	2	803	PHE	Peptide
2	3	172	THR	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	2	4714	0	4730	259	0
2	3	4745	0	4793	311	0
3	4	5081	0	5125	338	0
4	5	4962	0	4994	265	0
5	6	4742	0	4692	317	0
6	7	5432	0	5495	349	0
7	2	27	0	12	1	0
7	3	27	0	12	4	0
7	4	27	0	12	6	0
7	5	27	0	12	7	0
7	6	27	0	12	10	0
7	7	27	0	12	6	0
All	All	29838	0	29901	1676	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 1676 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)
2:3:653:ILE:CD1	4:5:402:ASP:HB3	1.36	1.53
2:3:653:ILE:HD13	4:5:402:ASP:CB	1.55	1.36
2:3:652:THR:C	2:3:654:PRO:HD3	1.52	1.28
2:3:653:ILE:CD1	4:5:402:ASP:CB	2.11	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:214:ARG:HG3	6:7:215:TYR:C	1.64	1.14

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	2	597/868 (69%)	544 (91%)	47 (8%)	6 (1%)	19	66
2	3	595/971 (61%)	548 (92%)	40 (7%)	7 (1%)	16	63
3	4	632/933 (68%)	554 (88%)	71 (11%)	7 (1%)	17	65
4	5	621/775 (80%)	586 (94%)	32 (5%)	3 (0%)	34	77
5	6	608/1017 (60%)	547 (90%)	52 (9%)	9 (2%)	13	59
6	7	681/845 (81%)	619 (91%)	52 (8%)	10 (2%)	13	59
All	All	3734/5409 (69%)	3398 (91%)	294 (8%)	42 (1%)	23	65

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	189	GLU
3	4	609	VAL
4	5	596	ILE
5	6	317	ILE
6	7	26	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	2	509/770 (66%)	509 (100%)	0	100 100
2	3	523/835 (63%)	523 (100%)	0	100 100
3	4	573/848 (68%)	572 (100%)	1 (0%)	95 98
4	5	566/688 (82%)	566 (100%)	0	100 100
5	6	497/886 (56%)	497 (100%)	0	100 100
6	7	609/753 (81%)	608 (100%)	1 (0%)	95 98
All	All	3277/4780 (69%)	3275 (100%)	2 (0%)	95 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	442	ILE
6	7	214	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
3	4	410	GLN
4	5	140	ASN
6	7	544	GLN
3	4	465	HIS
3	4	651	GLN

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)

6 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	$\#\|Z\| > 2$
7	ADP	2	2001	-	24,29,29	0.95	1 (4%)	23,45,45	1.95	2 (8%)
7	ADP	3	2001	-	24,29,29	1.00	1 (4%)	23,45,45	1.71	1 (4%)
7	ADP	4	2001	-	24,29,29	0.96	1 (4%)	23,45,45	1.70	2 (8%)
7	ADP	5	2001	-	24,29,29	0.97	1 (4%)	23,45,45	1.73	2 (8%)
7	ADP	6	2001	-	24,29,29	1.00	1 (4%)	23,45,45	1.85	2 (8%)
7	ADP	7	2001	-	24,29,29	0.98	1 (4%)	23,45,45	1.69	1 (4%)

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
7	ADP	2	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	3	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	4	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	5	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	6	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	7	2001	-	-	0/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	5	2001	ADP	C5-C4	2.82	1.46	1.40
7	4	2001	ADP	C5-C4	2.84	1.46	1.40
7	7	2001	ADP	C5-C4	2.88	1.47	1.40
7	2	2001	ADP	C5-C4	2.91	1.47	1.40
7	3	2001	ADP	C5-C4	2.92	1.47	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2	2001	ADP	N3-C2-N1	-7.35	123.10	128.87
7	6	2001	ADP	N3-C2-N1	-6.81	123.52	128.87
7	3	2001	ADP	N3-C2-N1	-6.35	123.88	128.87
7	5	2001	ADP	N3-C2-N1	-6.32	123.91	128.87
7	7	2001	ADP	N3-C2-N1	-6.30	123.92	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	2	2001	ADP	1	0
7	3	2001	ADP	4	0
7	4	2001	ADP	6	0
7	5	2001	ADP	7	0
7	6	2001	ADP	10	0
7	7	2001	ADP	6	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.