



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:31 am GMT

PDB ID : 4A54
Title : Structural basis of the Dcp1:Dcp2 mRNA decapping complex activation by Edc3 and Scd6
Authors : Fromm, S.A.; Truffault, V.; Kamenz, J.; Braun, J.E.; Hoffmann, N.A.; Izauralde, E.; Sprangers, R.
Deposited on : 2011-10-24

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

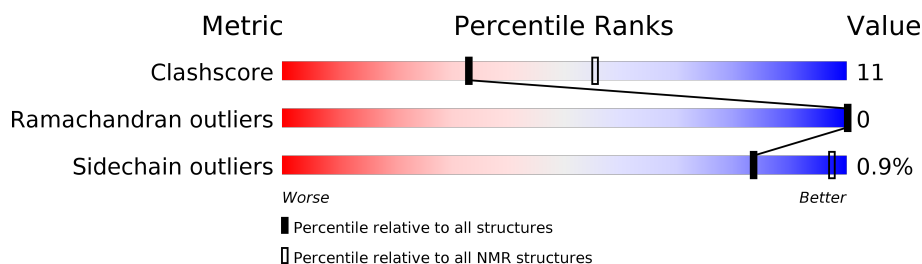
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	96	
2	B	52	

2 Ensemble composition and analysis

This entry contains 22 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:58, B:257-B:263 (64)	0.20	20

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 6, 12, 13, 15, 16, 17, 18, 20, 22
2	5, 7, 8, 11, 14, 19, 21
3	4, 10
Single-model clusters	9

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2239 atoms, of which 1124 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called EDC3.

Mol	Chain	Residues	Atoms						Trace
1	A	96	Total	C	H	N	O	S	0
			1496	456	756	128	152	4	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP O94752
A	0	GLY	-	EXPRESSION TAG	UNP O94752

- Molecule 2 is a protein called MRNA DECAPPING COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					Trace
2	B	52	Total	C	H	N	O	0
			743	229	368	61	85	

There are 2 discrepancies between the modelled and reference sequences:

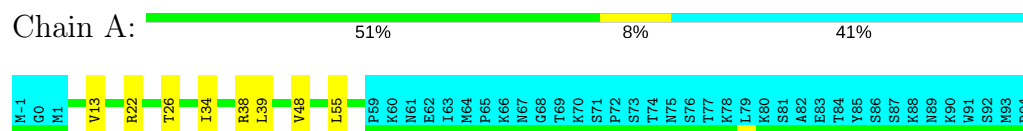
Chain	Residue	Modelled	Actual	Comment	Reference
B	240	GLY	-	EXPRESSION TAG	UNP O13828
B	241	ALA	-	EXPRESSION TAG	UNP O13828

4 Residue-property plots

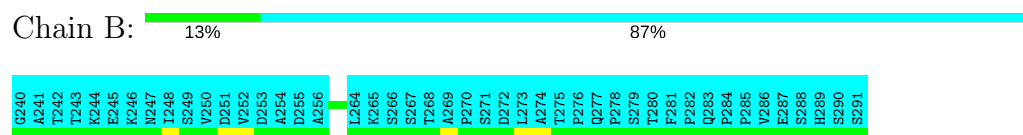
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: EDC3



- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

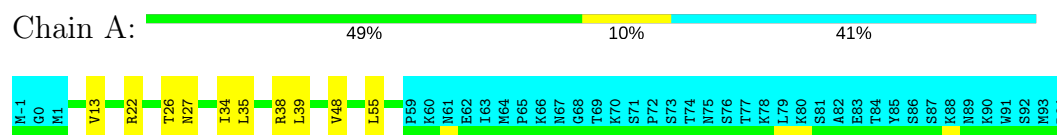


4.2 Scores per residue for each member of the ensemble

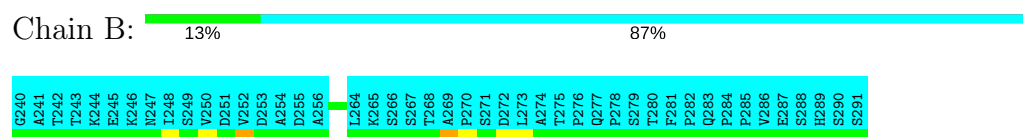
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: EDC3



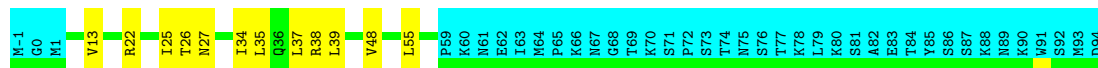
- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2



4.2.2 Score per residue for model 2

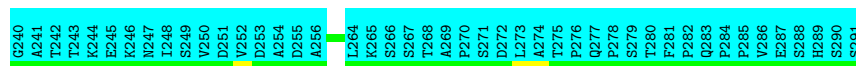
- Molecule 1: EDC3

Chain A: 



- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

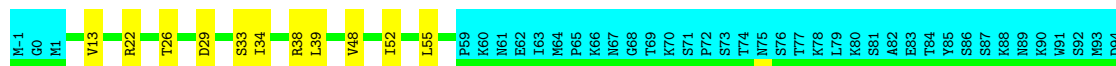
Chain B: 



4.2.3 Score per residue for model 3

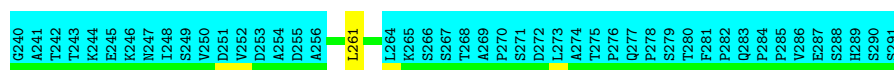
- Molecule 1: EDC3

Chain A: 



- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

Chain B: 



4.2.4 Score per residue for model 4

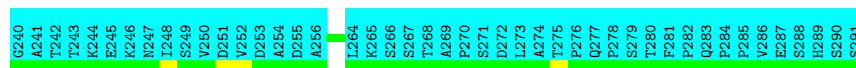
- Molecule 1: EDC3

Chain A: 



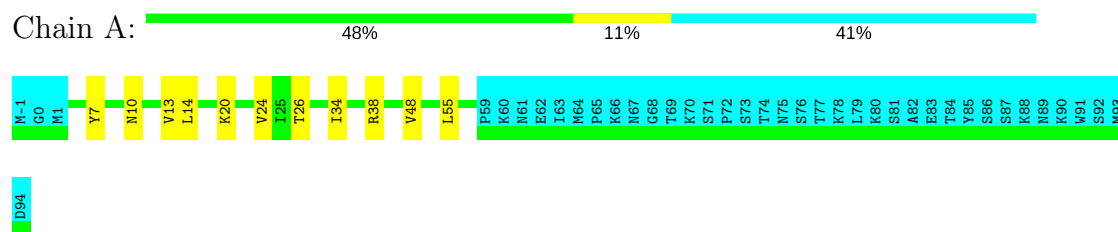
- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

Chain B: 

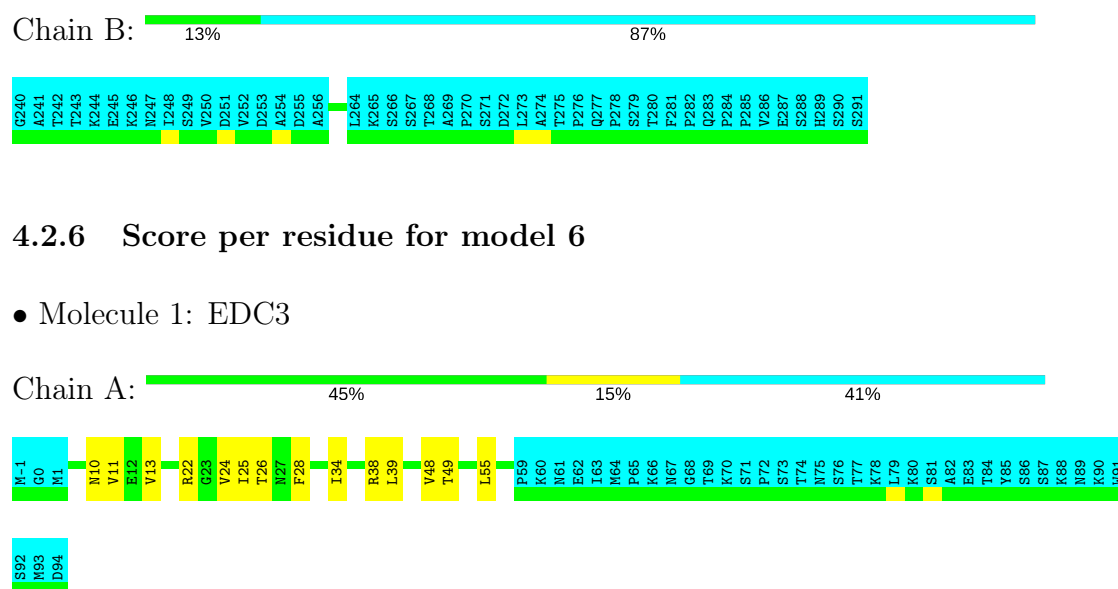


4.2.5 Score per residue for model 5

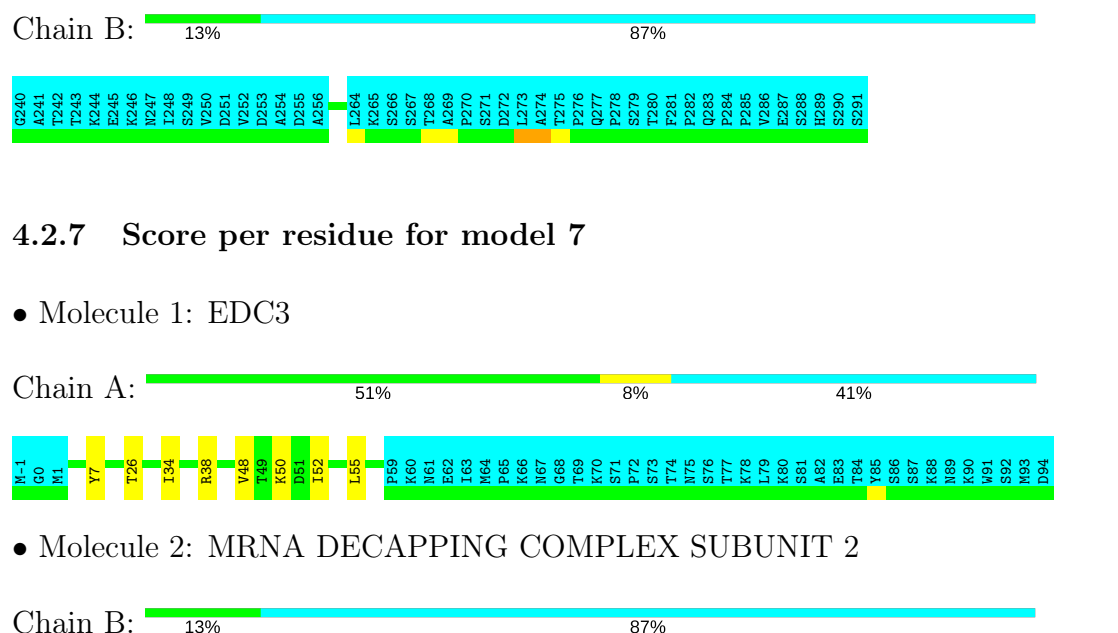
- Molecule 1: EDC3



- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

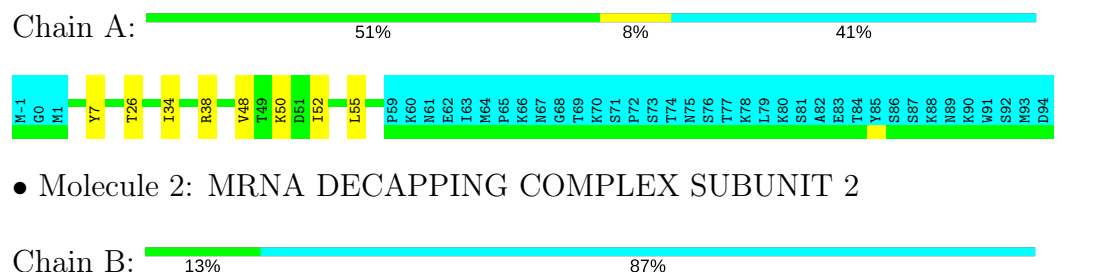


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

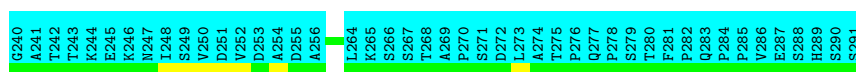


4.2.7 Score per residue for model 7

- Molecule 1: EDC3

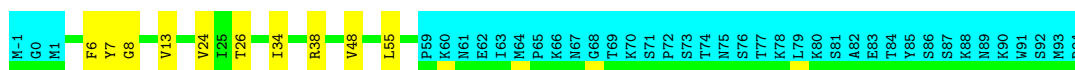


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

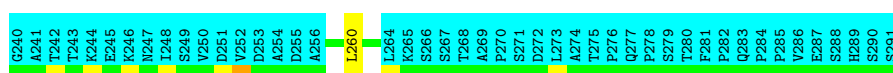


4.2.8 Score per residue for model 8

- Molecule 1: EDC3

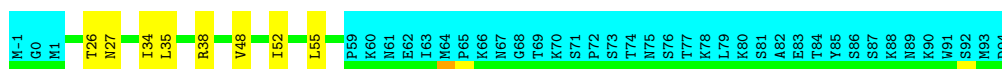


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

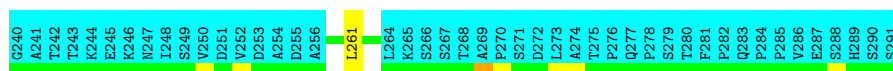


4.2.9 Score per residue for model 9

- Molecule 1: EDC3

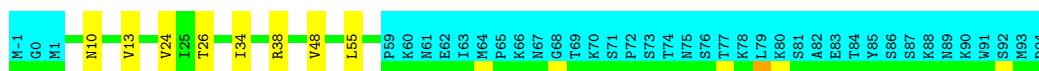


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2



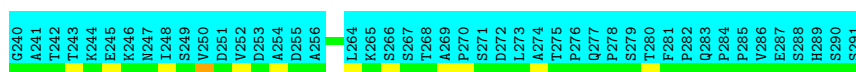
4.2.10 Score per residue for model 10

- Molecule 1: EDC3



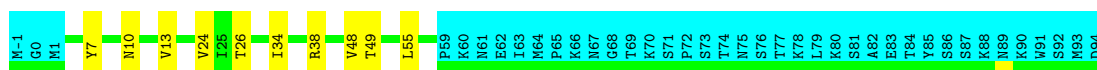
- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2



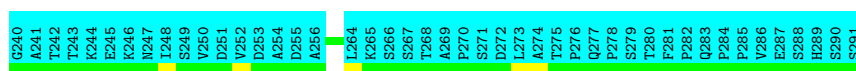


4.2.11 Score per residue for model 11

- Molecule 1: EDC3

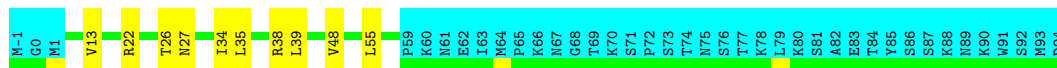


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2



4.2.12 Score per residue for model 12

- Molecule 1: EDC3

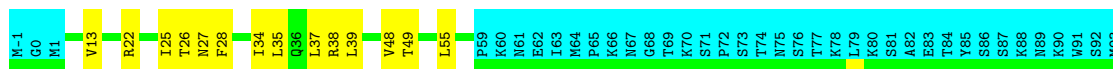


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

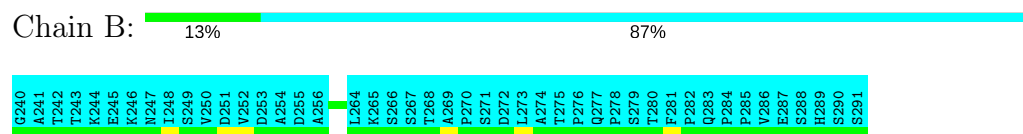


4.2.13 Score per residue for model 13

- Molecule 1: EDC3

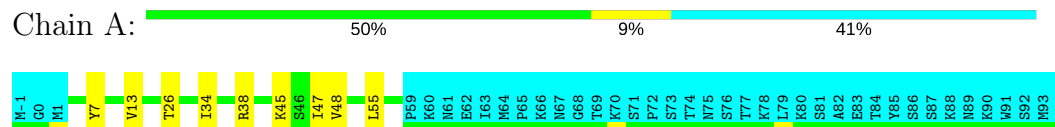


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

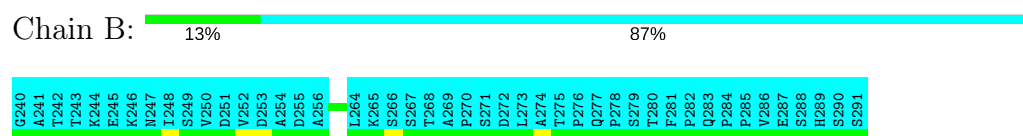


4.2.14 Score per residue for model 14

- Molecule 1: EDC3

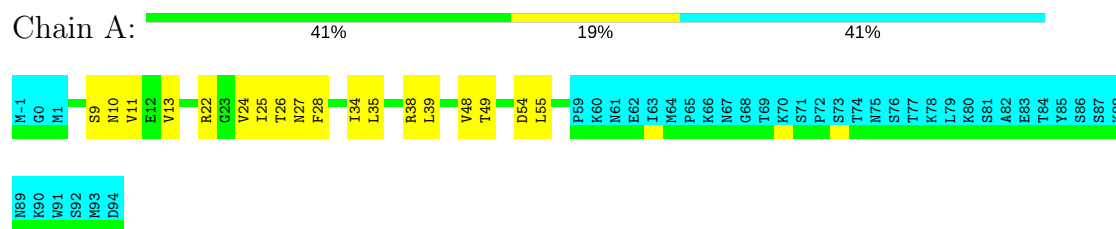


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

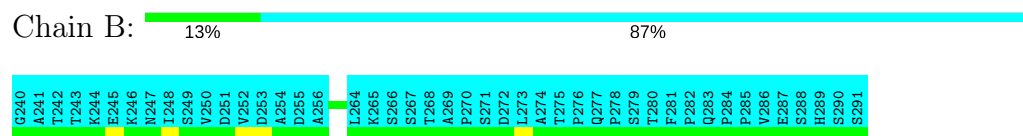


4.2.15 Score per residue for model 15

- Molecule 1: EDC3

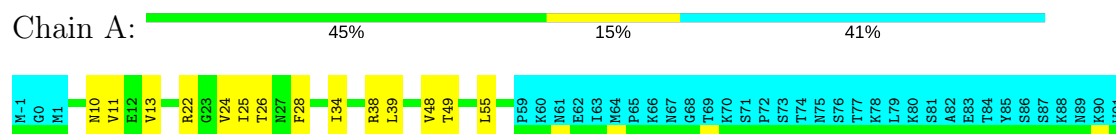


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2



4.2.16 Score per residue for model 16

- Molecule 1: EDC3



S92
M93
D94

- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

Chain B:  13% 87%

G240 A241 T242 T243 K244 E245 K246 N247 T248 S249 V250 D251 V252 D253 A254 D255 A256 L264 K265 S266 S267 T268 A269 P270 S271 D272 L273 A274 T275 P276 Q277 P278 S279 T280 F281 P282 Q283 P284 P285 V286 E287 S288 H289 S290 S291

4.2.17 Score per residue for model 17

- Molecule 1: EDC3

Chain A:  46% 14% 41%

M-1 G0 M1 N10 V11 E12 V13 R22 G23 V24 I25 T26 I34 R38 L39 V48 D54 L55 L58 P59 K60 N61 E62 I63 M64 K66 K67 T69 K70 S71 P72 T74 T75 N75 S76 T77 K78 L79 K80 S81 A82 E83 T84 Y85 S86 S87 K88 N89 K90 W91 S92

M93
D94

- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

Chain B:  13% 87%

G240 A241 T242 T243 K244 E245 K246 N247 T248 S249 V250 D251 V252 D253 A254 D255 A256 L264 K265 S266 S267 T268 A269 P270 S271 D272 L273 A274 T275 P276 Q277 P278 S279 T280 F281 P282 Q283 P284 P285 V286 E287 S288 H289 S290 S291

4.2.18 Score per residue for model 18

- Molecule 1: EDC3

Chain A:  48% 11% 41%

M-1 G0 M1 S9 R22 T25 T26 I34 L37 R38 L39 V48 I52 L55 P59 K60 N61 E62 I63 M64 K66 K67 T69 K70 S71 P72 T74 T75 N75 S76 T77 K78 L79 K80 S81 A82 E83 T84 Y85 S86 S87 K88 N89 K90 W91 S92 M93 D94

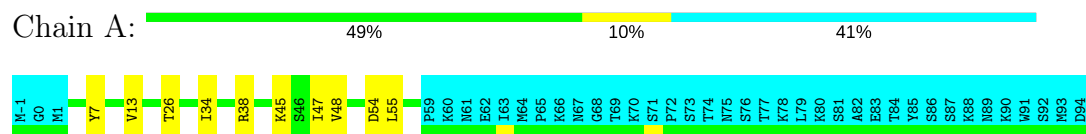
- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

Chain B:  12% 87%

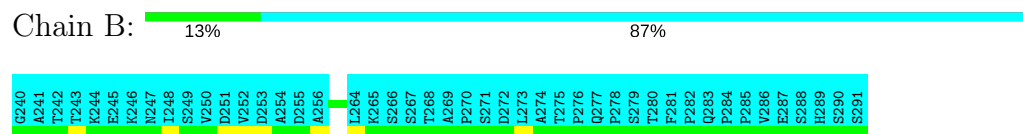
G240 A241 T242 T243 K244 E245 K246 N247 T248 S249 V250 D251 V252 D253 A254 D255 A256 L261 L264 K265 S266 S267 T268 A269 P270 S271 D272 L273 A274 T275 P276 Q277 P278 S279 T280 F281 P282 Q283 P284 P285 V286 E287 S288 H289 S290 S291

4.2.19 Score per residue for model 19

- Molecule 1: EDC3

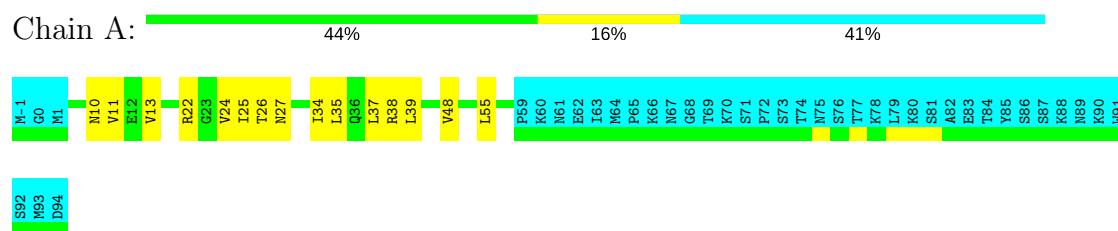


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

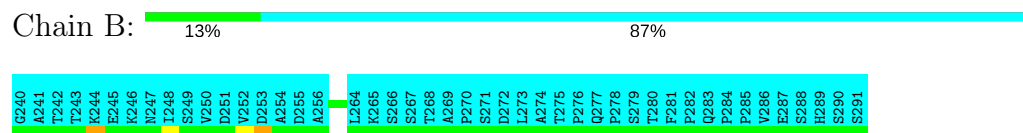


4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: EDC3

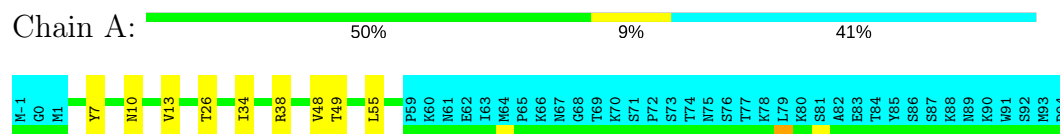


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

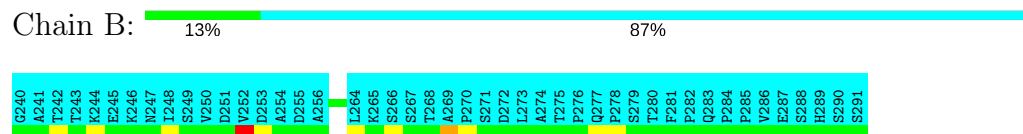


4.2.21 Score per residue for model 21

- Molecule 1: EDC3

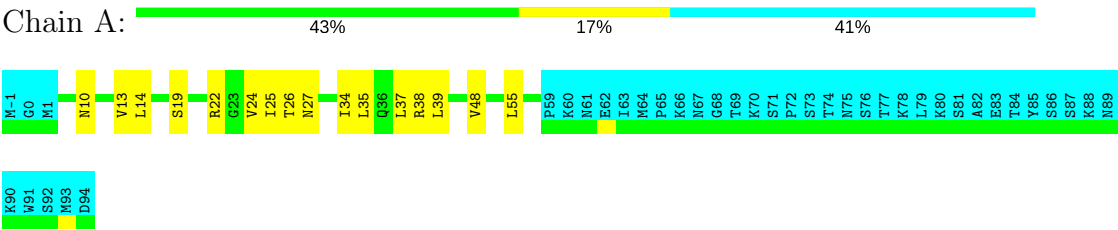


- Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2

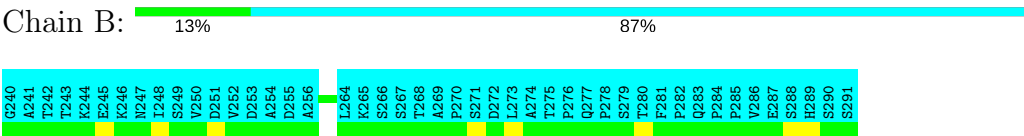


4.2.22 Score per residue for model 22

● Molecule 1: EDC3



● Molecule 2: MRNA DECAPPING COMPLEX SUBUNIT 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *XPLOR*.

Of the 50 calculated structures, 22 were deposited, based on the following criterion: *LOWEST ENERGY*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR 2.9.3	refinement	
SPARKY	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	4a54_cs.str
Number of chemical shift lists	1
Total number of shifts	466
Number of shifts mapped to atoms	466
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	440	451	451	10±2
2	B	51	56	56	0±1
All	All	10802	11154	11154	231

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 11.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HD12	1:A:48:VAL:HG22	0.98	1.36	8	22
1:A:34:ILE:HD13	1:A:48:VAL:HG13	0.76	1.57	12	22
1:A:10:ASN:ND2	1:A:24:VAL:HG22	0.68	2.03	11	8
1:A:10:ASN:CG	1:A:24:VAL:HG22	0.66	2.11	5	8
1:A:34:ILE:CD1	1:A:48:VAL:HG22	0.66	2.20	3	22
1:A:34:ILE:CD1	1:A:48:VAL:HG13	0.65	2.21	16	22
1:A:52:ILE:HG21	1:A:55:LEU:HD11	0.65	1.67	18	4
1:A:26:THR:HG21	1:A:38:ARG:HG3	0.62	1.70	1	4
1:A:10:ASN:OD1	1:A:24:VAL:HG22	0.60	1.96	17	3
1:A:13:VAL:HG22	1:A:55:LEU:CD2	0.60	2.26	10	18
1:A:45:LYS:HE2	1:A:47:ILE:HD11	0.58	1.74	19	1
1:A:26:THR:HG21	1:A:38:ARG:HB2	0.57	1.77	11	18
1:A:52:ILE:HG21	1:A:55:LEU:CD1	0.56	2.31	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:HD12	1:A:19:SER:O	0.55	2.02	22	1
1:A:11:VAL:HG21	1:A:25:ILE:HD11	0.54	1.79	16	4
1:A:13:VAL:HG22	1:A:55:LEU:HD23	0.54	1.79	10	2
1:A:26:THR:HG21	1:A:38:ARG:CG	0.54	2.33	1	3
1:A:9:SER:OG	1:A:25:ILE:HD12	0.52	2.04	4	3
1:A:13:VAL:CG1	1:A:52:ILE:HG23	0.52	2.35	3	1
1:A:13:VAL:HG13	1:A:55:LEU:CD2	0.50	2.37	1	15
1:A:10:ASN:OD1	1:A:24:VAL:HG13	0.48	2.09	10	1
1:A:55:LEU:HD12	2:B:261:LEU:HD13	0.47	1.85	3	3
1:A:25:ILE:HA	1:A:37:LEU:HD23	0.47	1.86	13	5
1:A:13:VAL:HG13	1:A:55:LEU:HD23	0.47	1.84	1	1
1:A:22:ARG:O	1:A:39:LEU:HD13	0.46	2.09	12	12
1:A:27:ASN:O	1:A:35:LEU:HD12	0.45	2.12	9	8
1:A:55:LEU:HD12	2:B:261:LEU:CD1	0.44	2.42	18	2
1:A:28:PHE:CE1	1:A:49:THR:HG21	0.42	2.49	16	4
1:A:13:VAL:HG13	1:A:55:LEU:HD21	0.42	1.92	2	3
1:A:14:LEU:HD13	1:A:20:LYS:HG2	0.42	1.91	5	1
1:A:12:GLU:HB2	1:A:58:LEU:HD11	0.41	1.91	17	1
1:A:45:LYS:HE3	1:A:47:ILE:HD11	0.41	1.92	14	1
1:A:29:ASP:O	1:A:33:SER:N	0.40	2.54	3	1
1:A:6:PHE:CE1	2:B:260:LEU:HD21	0.40	2.51	8	1
1:A:45:LYS:CE	1:A:47:ILE:HD11	0.40	2.47	14	1
1:A:8:GLY:O	1:A:24:VAL:HG13	0.40	2.16	8	1

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	57/96 (59%)	55±0 (96±0%)	2±0 (4±0%)	0±0 (0±0%)	100	100
2	B	7/52 (13%)	7±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1408/3256 (43%)	1364 (97%)	44 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 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 NMR 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	52/88 (59%)	51±1 (99±1%)	1±1 (1±1%)	81	97
2	B	7/46 (15%)	7±0 (100±0%)	0±0 (0±0%)	100	100
All	All	1298/2948 (44%)	1286 (99%)	12 (1%)	83	97

All 4 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	7	TYR	7
1	A	54	ASP	3
1	A	10	ASN	1
1	A	50	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 27% for the entire structure.

7.1 Chemical shift list 1

File name: 4a54_cs.str

Chemical shift list name: *edc3_15.bmr.b.csh*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	466
Number of shifts mapped to atoms	466
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	79	-0.27 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	75	0.14 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	75	0.30 ± 0.17	None needed (< 0.5 ppm)
^{15}N	71	-0.07 ± 0.30	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 46%, i.e. 354 atoms were assigned a chemical shift out of a possible 770. 12 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	228/320 (71%)	57/128 (45%)	114/128 (89%)	57/64 (89%)
Sidechain	126/424 (30%)	0/244 (0%)	121/159 (76%)	5/21 (24%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/26 (0%)	0/14 (0%)	0/12 (0%)	0/0 (—%)
Overall	354/770 (46%)	57/386 (15%)	235/299 (79%)	62/85 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 461 atoms were assigned a chemical shift out of a possible 1722. 13 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	296/722 (41%)	71/287 (25%)	154/296 (52%)	71/139 (51%)
Sidechain	165/938 (18%)	0/552 (0%)	160/348 (46%)	5/38 (13%)
Aromatic	0/62 (0%)	0/33 (0%)	0/27 (0%)	0/2 (0%)
Overall	461/1722 (27%)	71/872 (8%)	314/671 (47%)	76/179 (42%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

