



Full wwPDB NMR Structure Validation Report ⓘ

Feb 24, 2022 – 09:58 AM EST

PDB ID : 1Z1D
Title : Structural Model for the interaction between RPA32 C-terminal domain and SV40 T antigen origin binding domain.
Authors : Arunkumar, A.I.; Klimovich, V.; Jiang, X.; Ott, R.D.; Mizoue, L.; Fanning, E.; Chazin, W.J.
Deposited on : 2005-03-03

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

<https://www.wwpdb.org/validation/2017/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:

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

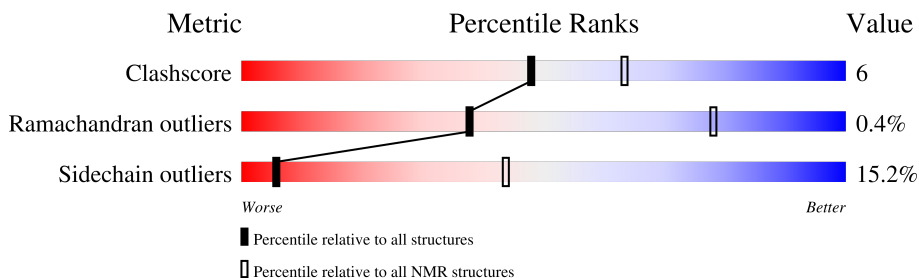
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	103	
2	B	131	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:205-A:266, B:1-B:131 (193)	0.57	9

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3193 atoms, of which 1590 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Replication protein A 32 kDa subunit.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	69	1061	332	524	94	109	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLY	-	cloning artifact	UNP P15927
A	169	SER	-	cloning artifact	UNP P15927
A	170	HIS	-	cloning artifact	UNP P15927
A	171	MET	-	cloning artifact	UNP P15927

- Molecule 2 is a protein called Large T antigen.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	131	2132	691	1066	178	192	5	0

There are 2 discrepancies between the modelled and reference sequences:

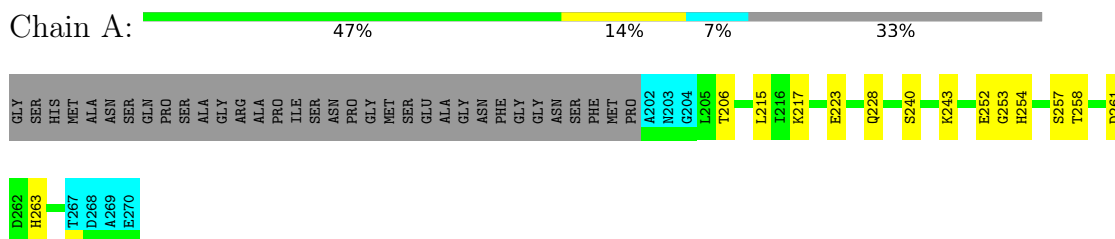
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	cloning artifact	UNP P03070
B	2	SER	-	cloning artifact	UNP P03070

4 Residue-property plots

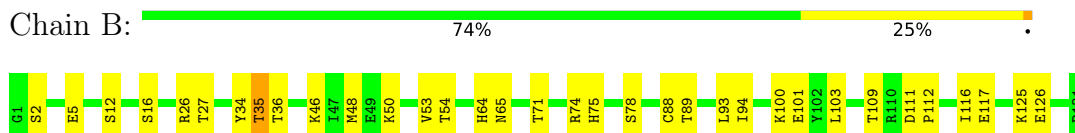
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Replication protein A 32 kDa subunit



- Molecule 2: Large T antigen

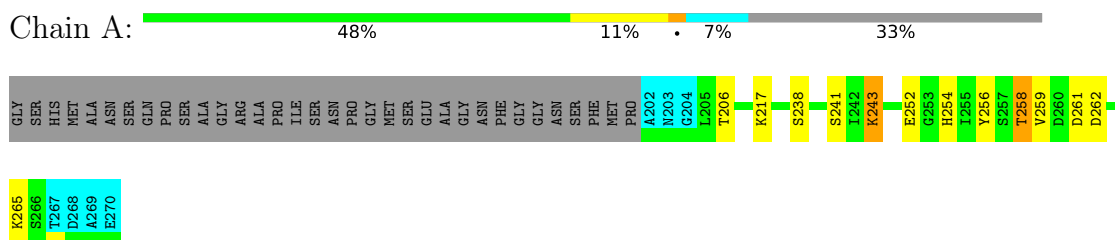


4.2 Scores per residue for each member of the ensemble

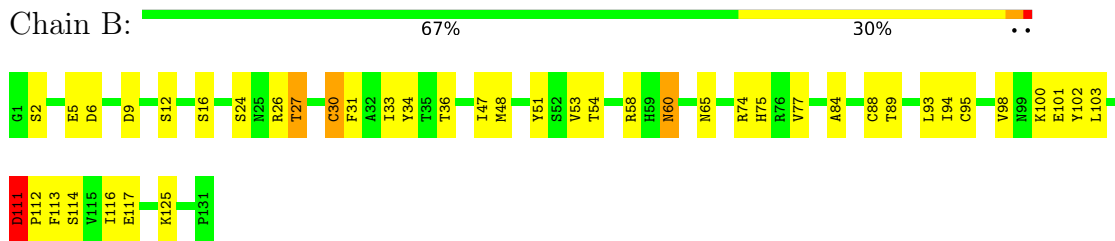
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Replication protein A 32 kDa subunit

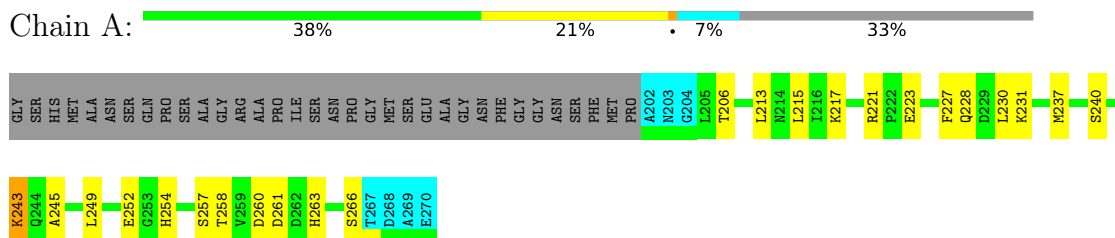


- Molecule 2: Large T antigen

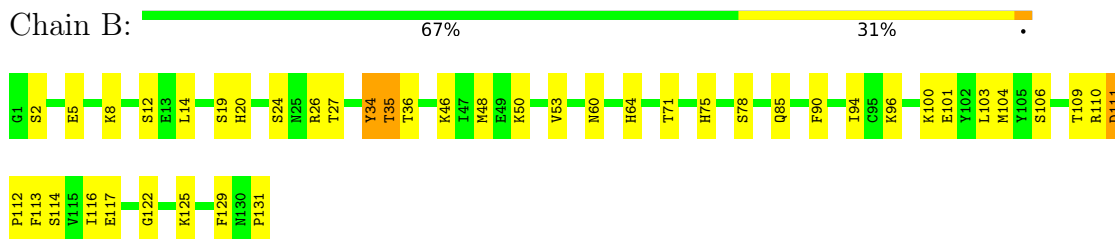


4.2.2 Score per residue for model 2

- Molecule 1: Replication protein A 32 kDa subunit

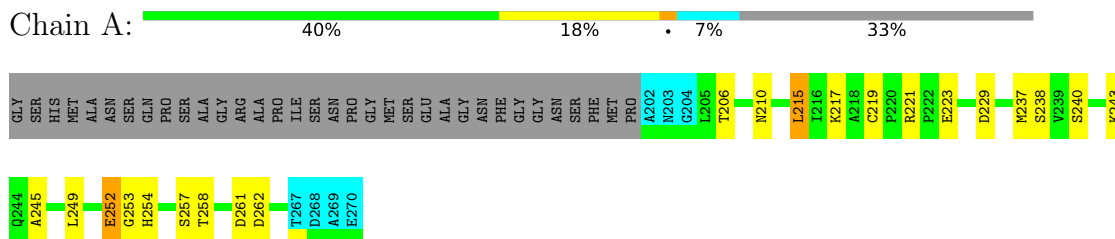


- Molecule 2: Large T antigen

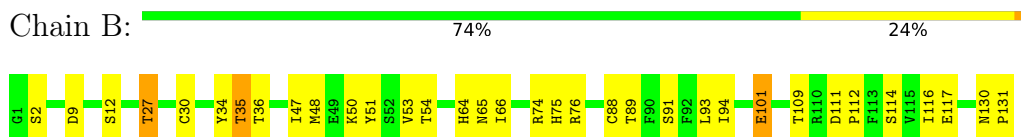


4.2.3 Score per residue for model 3

- Molecule 1: Replication protein A 32 kDa subunit

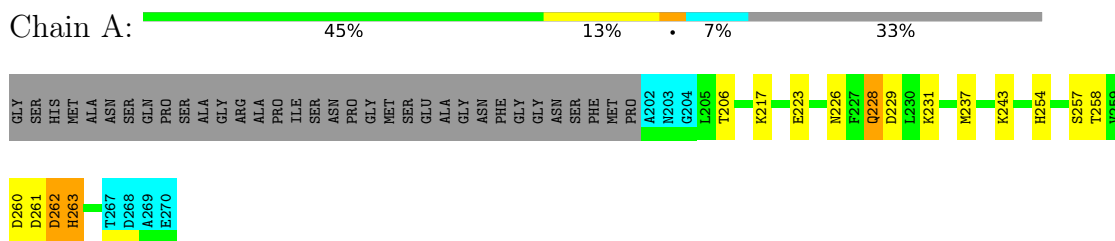


- Molecule 2: Large T antigen

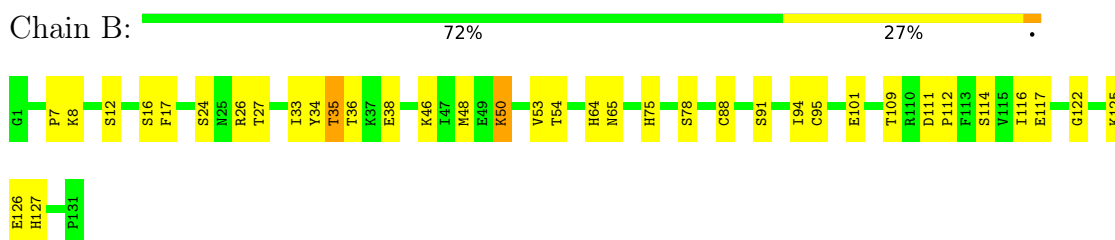


4.2.4 Score per residue for model 4

- Molecule 1: Replication protein A 32 kDa subunit

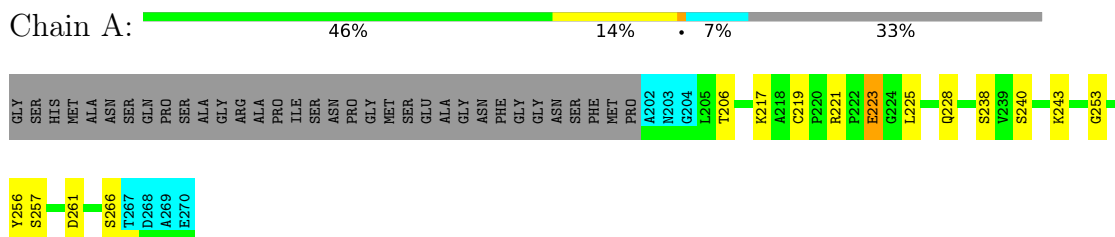


- Molecule 2: Large T antigen

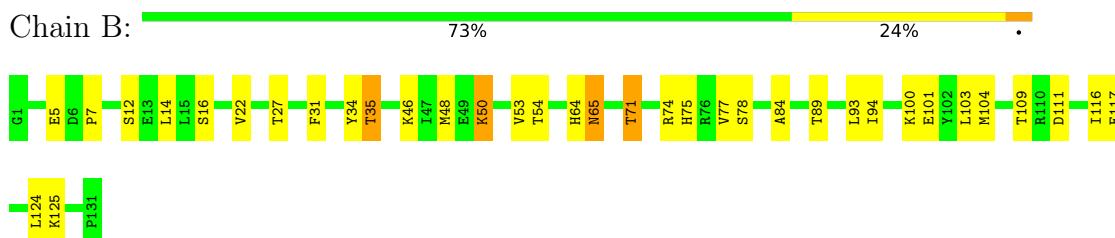


4.2.5 Score per residue for model 5

- Molecule 1: Replication protein A 32 kDa subunit



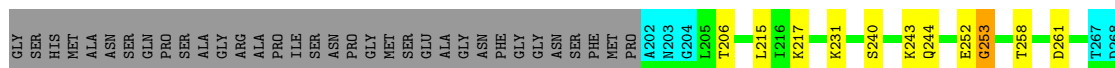
- Molecule 2: Large T antigen



4.2.6 Score per residue for model 6

- Molecule 1: Replication protein A 32 kDa subunit

Chain A:  50% 10% 7% 33%



 A269
E270

- Molecule 2: Large T antigen

Chain B:  69% 27%

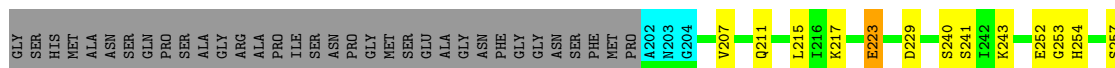


 P112
K126
E126
N130
P131

4.2.7 Score per residue for model 7

- Molecule 1: Replication protein A 32 kDa subunit

Chain A:  44% 16% 7% 33%



 T258
V259
D260
H263
S266
T267
D268
A269
E270

- Molecule 2: Large T antigen

Chain B:  73% 26%

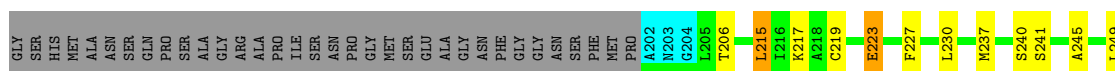


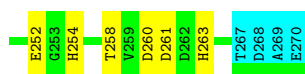
 F129
N130
P131

4.2.8 Score per residue for model 8

- Molecule 1: Replication protein A 32 kDa subunit

Chain A:  43% 16% 7% 33%





- Molecule 2: Large T antigen

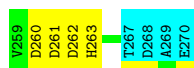
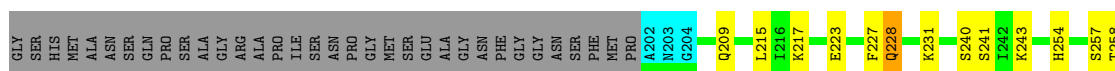
Chain B: 71% 27%



4.2.9 Score per residue for model 9 (medoid)

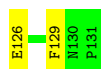
- Molecule 1: Replication protein A 32 kDa subunit

Chain A: 44% 16% 7% 33%



- Molecule 2: Large T antigen

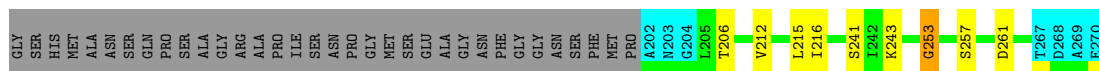
Chain B: 69% 29%



4.2.10 Score per residue for model 10

- Molecule 1: Replication protein A 32 kDa subunit

Chain A: 51% 8% 7% 33%



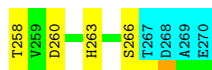
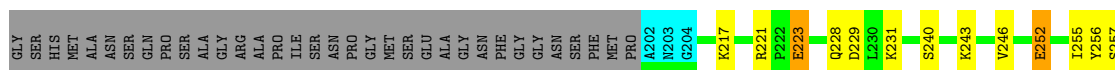
- Molecule 2: Large T antigen

Chain B: 73% 26%



4.2.11 Score per residue for model 11

- Molecule 1: Replication protein A 32 kDa subunit

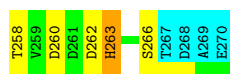
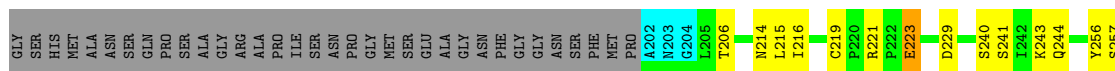


- Molecule 2: Large T antigen



4.2.12 Score per residue for model 12

- Molecule 1: Replication protein A 32 kDa subunit



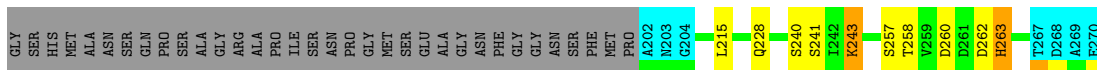
- Molecule 2: Large T antigen



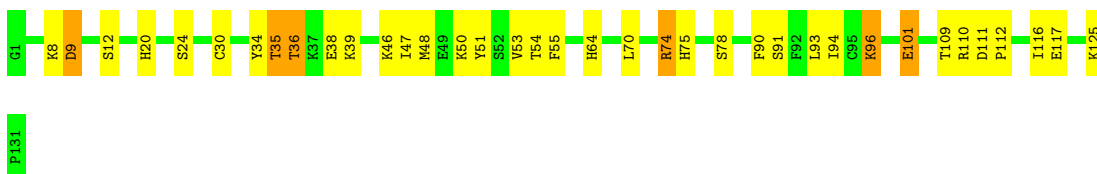


4.2.13 Score per residue for model 13

- Molecule 1: Replication protein A 32 kDa subunit

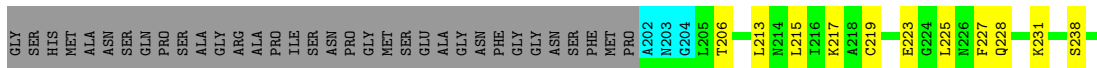


- Molecule 2: Large T antigen

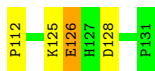
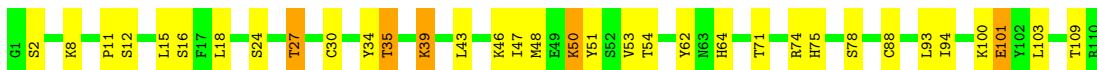


4.2.14 Score per residue for model 14

- Molecule 1: Replication protein A 32 kDa subunit



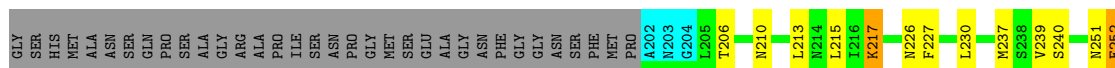
- Molecule 2: Large T antigen




4.2.15 Score per residue for model 15

- Molecule 1: Replication protein A 32 kDa subunit

Chain A: 



- Molecule 2: Large T antigen

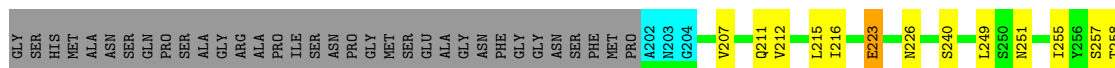
Chain B: 



4.2.16 Score per residue for model 16

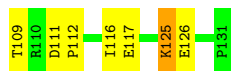
- Molecule 1: Replication protein A 32 kDa subunit

Chain A: 



- Molecule 2: Large T antigen

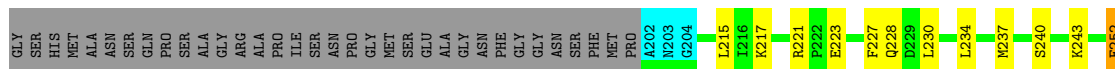
Chain B: 



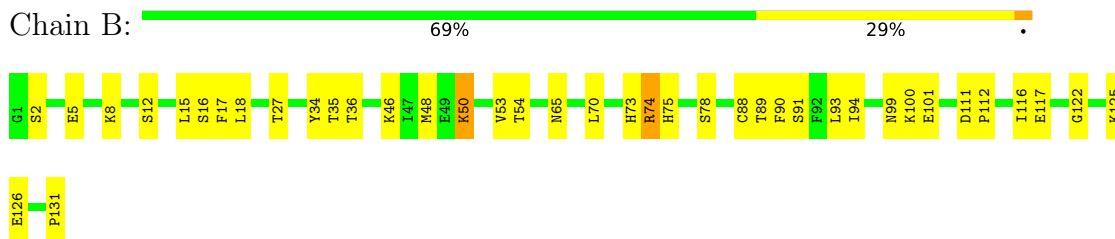
4.2.17 Score per residue for model 17

- Molecule 1: Replication protein A 32 kDa subunit

Chain A: 

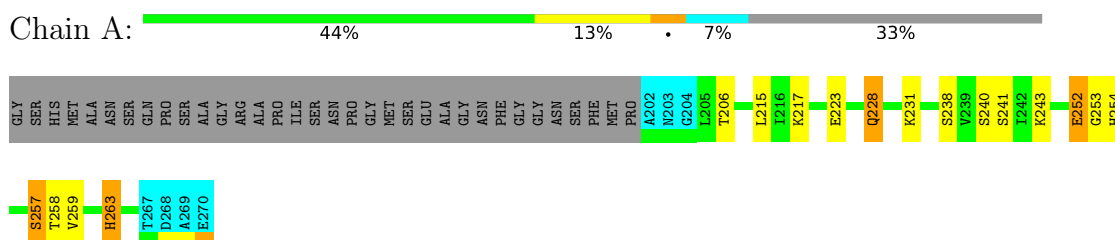


- Molecule 2: Large T antigen



4.2.18 Score per residue for model 18

- Molecule 1: Replication protein A 32 kDa subunit

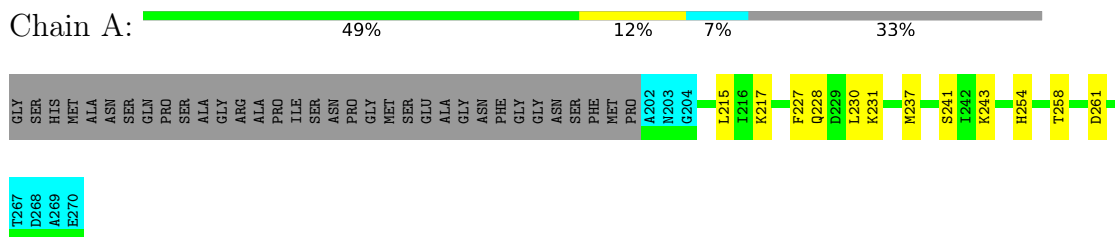


- Molecule 2: Large T antigen

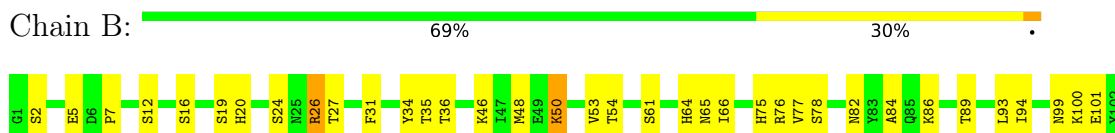


4.2.19 Score per residue for model 19

- Molecule 1: Replication protein A 32 kDa subunit



- Molecule 2: Large T antigen

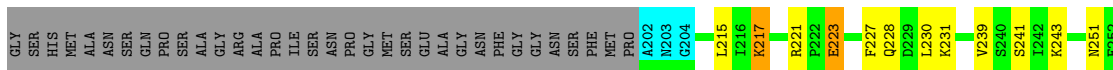




4.2.20 Score per residue for model 20

- Molecule 1: Replication protein A 32 kDa subunit

Chain A: 43% 16% 7% 33%



- Molecule 2: Large T antigen

Chain B: 70% 27%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Rigid body docking, Semi-flexible simulated annealing, Refinement using explicit water.*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with favorable non-bond energy.*

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

Software name	Classification	Version
HADDOCK	structure solution	1.3
HADDOCK	refinement	1.3

No chemical shift data was provided.

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	490	488	485	5±2
2	B	1066	1066	1060	16±3
All	All	31120	31080	30900	393

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:111:ASP:HB3	2:B:112:PRO:HD3	0.82	1.51	18	19
1:A:228:GLN:HA	1:A:231:LYS:HE2	0.80	1.51	11	7
2:B:125:LYS:HA	2:B:125:LYS:HE2	0.71	1.59	16	13
2:B:100:LYS:HB3	2:B:103:LEU:HB2	0.66	1.68	5	12
2:B:34:TYR:HB3	2:B:94:ILE:HB	0.66	1.66	11	15
1:A:227:PHE:HA	1:A:230:LEU:HD12	0.66	1.68	20	6
2:B:48:MET:HA	2:B:53:VAL:HG22	0.65	1.69	8	17
2:B:111:ASP:HB3	2:B:112:PRO:CD	0.65	2.22	2	4
2:B:116:ILE:HG22	2:B:117:GLU:HG3	0.63	1.69	11	13
1:A:252:GLU:HB3	1:A:254:HIS:HD2	0.63	1.54	18	3
2:B:9:ASP:HA	2:B:94:ILE:HG21	0.62	1.71	13	3
1:A:260:ASP:HB3	1:A:263:HIS:HB2	0.62	1.71	14	9
1:A:246:VAL:HA	1:A:255:ILE:HD11	0.62	1.70	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:11:PRO:HB3	2:B:62:TYR:HE2	0.62	1.54	14	2
2:B:29:ALA:HB2	2:B:74:ARG:HE	0.62	1.54	20	1
2:B:34:TYR:HD2	2:B:94:ILE:HD12	0.62	1.54	19	2
2:B:111:ASP:CB	2:B:112:PRO:HD3	0.62	2.25	1	2
2:B:126:GLU:HB2	2:B:131:PRO:HG3	0.60	1.71	8	2
2:B:35:THR:HG21	2:B:39:LYS:HD2	0.60	1.71	14	2
1:A:217:LYS:HB3	1:A:266:SER:HB2	0.60	1.73	15	1
2:B:88:CYS:SG	2:B:93:LEU:HB3	0.60	2.37	14	5
1:A:252:GLU:HB3	1:A:254:HIS:CD2	0.58	2.34	18	6
1:A:252:GLU:HA	2:B:26:ARG:CZ	0.57	2.29	2	1
1:A:253:GLY:HA3	2:B:27:THR:HB	0.57	1.77	20	1
2:B:15:LEU:HA	2:B:18:LEU:HD12	0.57	1.76	14	2
1:A:221:ARG:HB3	1:A:223:GLU:OE2	0.56	2.01	12	3
2:B:7:PRO:HD2	2:B:64:HIS:HE1	0.56	1.60	18	4
2:B:26:ARG:HG3	2:B:28:LEU:HG	0.56	1.75	12	1
2:B:27:THR:HB	2:B:74:ARG:HB3	0.56	1.77	14	1
1:A:253:GLY:O	2:B:27:THR:HB	0.55	2.01	15	1
2:B:39:LYS:HE3	2:B:87:LEU:HB3	0.55	1.78	16	1
2:B:27:THR:HG23	2:B:76:ARG:HD3	0.55	1.77	3	1
2:B:34:TYR:CE1	2:B:64:HIS:HB2	0.55	2.37	2	1
2:B:61:SER:HB3	2:B:66:ILE:HD11	0.55	1.79	19	5
1:A:252:GLU:HA	2:B:26:ARG:NH1	0.54	2.16	18	3
1:A:261:ASP:HB3	2:B:131:PRO:HG3	0.54	1.79	3	1
2:B:46:LYS:O	2:B:50:LYS:HB2	0.54	2.03	17	11
2:B:60:ASN:O	2:B:113:PHE:HA	0.53	2.03	1	3
1:A:256:TYR:HB3	2:B:74:ARG:NH2	0.53	2.18	1	1
2:B:14:LEU:HD22	2:B:104:MET:HG3	0.53	1.80	2	3
2:B:27:THR:HG21	2:B:74:ARG:HB3	0.53	1.79	1	1
2:B:30:CYS:HB2	2:B:98:VAL:HB	0.53	1.80	1	1
1:A:213:LEU:HD11	1:A:254:HIS:HB3	0.53	1.81	2	2
1:A:223:GLU:HB3	1:A:263:HIS:NE2	0.52	2.20	8	2
2:B:65:ASN:HD21	2:B:116:ILE:HD11	0.52	1.65	12	3
1:A:257:SER:HA	1:A:263:HIS:O	0.52	2.04	18	1
1:A:245:ALA:O	1:A:249:LEU:HG	0.51	2.05	2	3
2:B:17:PHE:HB3	2:B:100:LYS:HB2	0.51	1.81	9	3
1:A:260:ASP:HB3	1:A:263:HIS:CB	0.51	2.36	14	3
2:B:7:PRO:HD2	2:B:64:HIS:CE1	0.51	2.41	18	4
2:B:35:THR:O	2:B:64:HIS:HB3	0.51	2.06	13	14
2:B:31:PHE:HE1	2:B:77:VAL:HG22	0.50	1.65	11	3
2:B:26:ARG:O	2:B:76:ARG:HA	0.50	2.06	19	1
2:B:88:CYS:HA	2:B:91:SER:O	0.50	2.07	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:253:GLY:CA	2:B:74:ARG:HG2	0.50	2.36	14	1
1:A:228:GLN:HA	1:A:231:LYS:HE3	0.50	1.83	18	1
1:A:221:ARG:HB3	1:A:223:GLU:OE1	0.49	2.06	11	3
2:B:34:TYR:CD1	2:B:94:ILE:HD12	0.49	2.42	9	4
2:B:53:VAL:HG12	2:B:71:THR:HG23	0.49	1.82	5	3
2:B:12:SER:HA	2:B:15:LEU:HD12	0.49	1.84	11	2
2:B:82:ASN:O	2:B:86:LYS:HG3	0.49	2.07	19	1
2:B:22:VAL:O	2:B:77:VAL:HB	0.49	2.07	12	4
2:B:34:TYR:HD1	2:B:66:ILE:HG12	0.49	1.67	19	1
1:A:219:CYS:SG	1:A:225:LEU:HD13	0.48	2.48	14	2
2:B:42:LEU:HB3	2:B:46:LYS:HE2	0.48	1.85	20	1
1:A:249:LEU:HB3	1:A:255:ILE:HG12	0.48	1.85	16	1
2:B:33:ILE:HG12	2:B:95:CYS:SG	0.48	2.49	11	3
2:B:11:PRO:HB3	2:B:62:TYR:CE2	0.48	2.42	14	1
2:B:18:LEU:HD22	2:B:96:LYS:HB3	0.48	1.86	10	1
1:A:253:GLY:HA2	2:B:74:ARG:NH1	0.48	2.24	18	3
2:B:68:PHE:CE1	2:B:98:VAL:HG21	0.47	2.44	7	1
1:A:227:PHE:HB3	1:A:262:ASP:OD1	0.47	2.09	9	1
2:B:124:LEU:HB3	2:B:129:PHE:CZ	0.47	2.44	10	2
1:A:253:GLY:CA	2:B:74:ARG:HG3	0.47	2.40	5	1
1:A:243:LYS:HA	1:A:243:LYS:HE2	0.47	1.87	13	3
2:B:34:TYR:CD2	2:B:94:ILE:HD12	0.47	2.45	8	7
1:A:212:VAL:O	1:A:216:ILE:HG13	0.47	2.09	10	2
1:A:253:GLY:HA2	2:B:74:ARG:HG3	0.47	1.85	5	2
1:A:216:ILE:HB	1:A:266:SER:OG	0.47	2.10	12	1
2:B:84:ALA:HB1	2:B:93:LEU:HD11	0.47	1.86	19	6
1:A:223:GLU:HB3	1:A:263:HIS:CE1	0.47	2.45	16	2
2:B:55:PHE:HB2	2:B:120:LEU:HD12	0.47	1.87	20	1
2:B:30:CYS:SG	2:B:101:GLU:HB3	0.47	2.50	14	4
1:A:257:SER:HB3	1:A:260:ASP:O	0.47	2.09	4	1
2:B:124:LEU:O	2:B:125:LYS:HE2	0.46	2.09	15	2
1:A:258:THR:HG21	1:A:265:LYS:HD3	0.46	1.88	1	1
2:B:127:HIS:HA	2:B:131:PRO:HG3	0.46	1.88	20	1
1:A:227:PHE:HE1	1:A:239:VAL:HG13	0.46	1.71	15	1
1:A:253:GLY:HA2	2:B:74:ARG:HG2	0.46	1.88	20	1
2:B:126:GLU:HB2	2:B:131:PRO:HA	0.46	1.87	11	1
2:B:74:ARG:HD2	2:B:74:ARG:N	0.46	2.26	11	1
1:A:252:GLU:HA	2:B:26:ARG:NH2	0.45	2.26	11	1
2:B:126:GLU:H	2:B:126:GLU:CD	0.45	2.15	14	3
2:B:85:GLN:HA	2:B:93:LEU:HD22	0.45	1.88	8	1
2:B:29:ALA:HB2	2:B:74:ARG:HG2	0.45	1.88	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:252:GLU:HA	2:B:26:ARG:HH12	0.45	1.70	18	1
2:B:58:ARG:HB3	2:B:116:ILE:HD12	0.45	1.89	20	1
1:A:215:LEU:O	1:A:219:CYS:HB2	0.45	2.11	8	2
2:B:36:THR:HB	2:B:38:GLU:OE1	0.45	2.11	13	1
2:B:58:ARG:NH2	2:B:116:ILE:HG21	0.44	2.27	1	1
2:B:85:GLN:O	2:B:88:CYS:HB2	0.44	2.12	12	2
2:B:30:CYS:SG	2:B:70:LEU:HG	0.44	2.52	6	2
2:B:39:LYS:NZ	2:B:93:LEU:HB2	0.44	2.26	18	4
2:B:25:ASN:OD1	2:B:76:ARG:HD3	0.44	2.12	15	1
1:A:253:GLY:HA3	2:B:27:THR:O	0.44	2.13	7	2
2:B:13:GLU:H	2:B:13:GLU:CD	0.44	2.16	8	1
1:A:207:VAL:O	1:A:211:GLN:HG3	0.44	2.13	16	1
2:B:111:ASP:CB	2:B:112:PRO:CD	0.44	2.96	2	2
2:B:33:ILE:HB	2:B:67:LEU:HB3	0.44	1.89	11	2
2:B:37:LYS:HG3	2:B:38:GLU:OE1	0.44	2.13	18	1
2:B:129:PHE:O	2:B:131:PRO:HD3	0.44	2.13	7	2
1:A:226:ASN:HB2	1:A:229:ASP:OD2	0.43	2.13	4	1
2:B:51:TYR:HB3	2:B:71:THR:HG21	0.43	1.90	12	1
2:B:34:TYR:CD1	2:B:66:ILE:HG12	0.43	2.48	3	1
2:B:53:VAL:HG12	2:B:71:THR:HG22	0.43	1.91	2	2
2:B:125:LYS:HB2	2:B:127:HIS:CE1	0.43	2.49	4	1
2:B:35:THR:HG21	2:B:39:LYS:HD3	0.43	1.89	7	1
2:B:33:ILE:HD12	2:B:67:LEU:HD23	0.43	1.89	10	1
2:B:34:TYR:HE1	2:B:64:HIS:HB2	0.43	1.71	2	1
2:B:20:HIS:HA	2:B:96:LYS:HD3	0.43	1.90	13	2
2:B:43:LEU:HA	2:B:46:LYS:HB2	0.43	1.91	7	3
1:A:228:GLN:HG3	1:A:229:ASP:N	0.42	2.30	11	1
2:B:19:SER:O	2:B:20:HIS:HB2	0.42	2.15	19	2
2:B:31:PHE:HB2	2:B:69:PHE:CZ	0.42	2.49	16	2
2:B:5:GLU:O	2:B:7:PRO:HD3	0.42	2.14	10	1
2:B:25:ASN:HA	2:B:76:ARG:CZ	0.42	2.45	16	1
2:B:31:PHE:HE1	2:B:77:VAL:HG13	0.42	1.73	1	1
2:B:29:ALA:HB2	2:B:74:ARG:HD2	0.42	1.91	16	1
1:A:207:VAL:HG12	1:A:211:GLN:HE21	0.42	1.75	7	1
1:A:227:PHE:HE2	1:A:239:VAL:HG13	0.41	1.75	20	1
1:A:253:GLY:HA2	2:B:74:ARG:CZ	0.41	2.45	10	2
2:B:47:ILE:HG23	2:B:51:TYR:HD2	0.41	1.76	12	5
1:A:253:GLY:O	2:B:74:ARG:HB3	0.41	2.16	3	1
1:A:226:ASN:HA	1:A:262:ASP:O	0.41	2.15	15	2
2:B:15:LEU:HD23	2:B:18:LEU:HD12	0.41	1.91	17	2
2:B:106:SER:O	2:B:110:ARG:HG3	0.41	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:256:TYR:HB3	2:B:74:ARG:HH12	0.41	1.73	5	1
2:B:55:PHE:HD2	2:B:70:LEU:HD13	0.41	1.74	13	1
1:A:243:LYS:HZ3	2:B:131:PRO:C	0.41	2.19	18	1
1:A:219:CYS:SG	1:A:221:ARG:HG3	0.41	2.56	3	2
1:A:227:PHE:HB2	1:A:264:PHE:HE2	0.41	1.75	14	1
2:B:13:GLU:CD	2:B:13:GLU:H	0.40	2.18	15	1
1:A:256:TYR:HB3	2:B:74:ARG:NH1	0.40	2.31	5	2
2:B:44:TYR:O	2:B:48:MET:HB2	0.40	2.16	6	1
2:B:17:PHE:CD1	2:B:103:LEU:HB3	0.40	2.51	10	1
2:B:48:MET:HA	2:B:53:VAL:CG2	0.40	2.46	7	1
2:B:35:THR:HA	2:B:92:PHE:CZ	0.40	2.50	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	62/103 (60%)	58±1 (93±2%)	4±1 (6±2%)	0±0 (0±1%)	44	80
2	B	129/131 (98%)	115±2 (89±2%)	13±2 (10±2%)	1±1 (0±1%)	38	78
All	All	3820/4680 (82%)	3462 (91%)	343 (9%)	15 (0%)	38	78

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	111	ASP	3
2	B	122	GLY	3
1	A	253	GLY	2
2	B	2	SER	1
2	B	72	PRO	1
2	B	112	PRO	1
1	A	259	VAL	1
1	A	258	THR	1
2	B	90	PHE	1
2	B	61	SER	1

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	57/85 (67%)	47±2 (83±3%)	10±2 (17±3%)	5	40
2	B	119/119 (100%)	102±2 (86±2%)	17±2 (14±2%)	6	45
All	All	3520/4080 (86%)	2984 (85%)	536 (15%)	6	44

All 81 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)
2	B	75	HIS	20
2	B	101	GLU	20
2	B	27	THR	19
2	B	12	SER	18
2	B	54	THR	18
2	B	78	SER	18
1	A	258	THR	17
2	B	36	THR	17
1	A	215	LEU	16
2	B	35	THR	16
1	A	243	LYS	15
1	A	257	SER	15
1	A	217	LYS	14
1	A	240	SER	14
2	B	16	SER	13
1	A	206	THR	12
2	B	2	SER	12
2	B	65	ASN	12
2	B	89	THR	12
2	B	109	THR	12
2	B	5	GLU	11
1	A	223	GLU	11
2	B	50	LYS	11
1	A	241	SER	10
1	A	261	ASP	10
2	B	8	LYS	10
2	B	24	SER	8
1	A	266	SER	8

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Mol	Chain	Res	Type	Models (Total)
1	A	237	MET	7
2	B	126	GLU	7
2	B	71	THR	7
2	B	9	ASP	6
2	B	114	SER	6
1	A	252	GLU	6
1	A	228	GLN	6
1	A	238	SER	5
1	A	262	ASP	5
2	B	26	ARG	5
2	B	99	ASN	5
2	B	125	LYS	4
1	A	263	HIS	4
2	B	6	ASP	3
2	B	102	TYR	3
2	B	85	GLN	3
2	B	90	PHE	3
1	A	229	ASP	3
2	B	93	LEU	3
2	B	73	HIS	3
2	B	74	ARG	3
2	B	91	SER	3
1	A	251	ASN	3
1	A	259	VAL	2
2	B	60	ASN	2
2	B	111	ASP	2
1	A	210	ASN	2
2	B	130	ASN	2
1	A	254	HIS	2
2	B	17	PHE	2
2	B	38	GLU	2
1	A	244	GLN	2
2	B	39	LYS	2
2	B	88	CYS	2
2	B	96	LYS	2
2	B	110	ARG	2
2	B	129	PHE	2
2	B	30	CYS	1
2	B	19	SER	1
2	B	34	TYR	1
2	B	124	LEU	1
1	A	231	LYS	1

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Mol	Chain	Res	Type	Models (Total)
2	B	55	PHE	1
1	A	209	GLN	1
2	B	92	PHE	1
1	A	214	ASN	1
2	B	128	ASP	1
2	B	103	LEU	1
1	A	226	ASN	1
2	B	13	GLU	1
2	B	63	ASN	1
1	A	234	LEU	1
2	B	70	LEU	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 monosaccharides 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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided