wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 03:02 am BST

PDB ID	:	1N4M
Title	:	Structure of Rb tumor suppressor bound to the transactivation domain of E2F-2
Authors	:	Lee, C.; Chang, J.H.; Lee, H.S.; Cho, Y.
Deposited on	:	2002-10-31
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

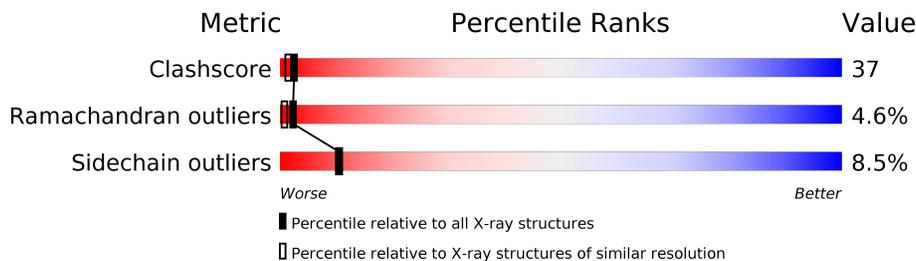|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Percentile Ranks	Value
Clashscore		37
Ramachandran outliers		4.6%
Sidechain outliers		8.5%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	45% 44% 10% •
1	B	345	47% 45% 6% •
2	C	18	61% 33% 6%
2	D	18	39% 56% 6%
2	E	18	17% 17% 22% 11% 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6249 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Retinoblastoma Pocket.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total 2829	C 1817	N 477	O 515	S 20	0	0	0
1	B	338	Total 2780	C 1790	N 468	O 502	S 20	0	0	0

- Molecule 2 is a protein called Transcription factor E2F2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	18	Total 143	C 91	N 19	O 33	0	0	0
2	D	18	Total 143	C 91	N 19	O 33	0	0	0
2	E	12	Total 93	C 59	N 13	O 21	0	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total 144	O 144	0	0
3	B	100	Total 100	O 100	0	0
3	C	4	Total 4	O 4	0	0
3	D	6	Total 6	O 6	0	0
3	E	7	Total 7	O 7	0	0

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 the various outlier classes 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.

Note EDS was not executed.

• Molecule 1: Retinoblastoma Pocket
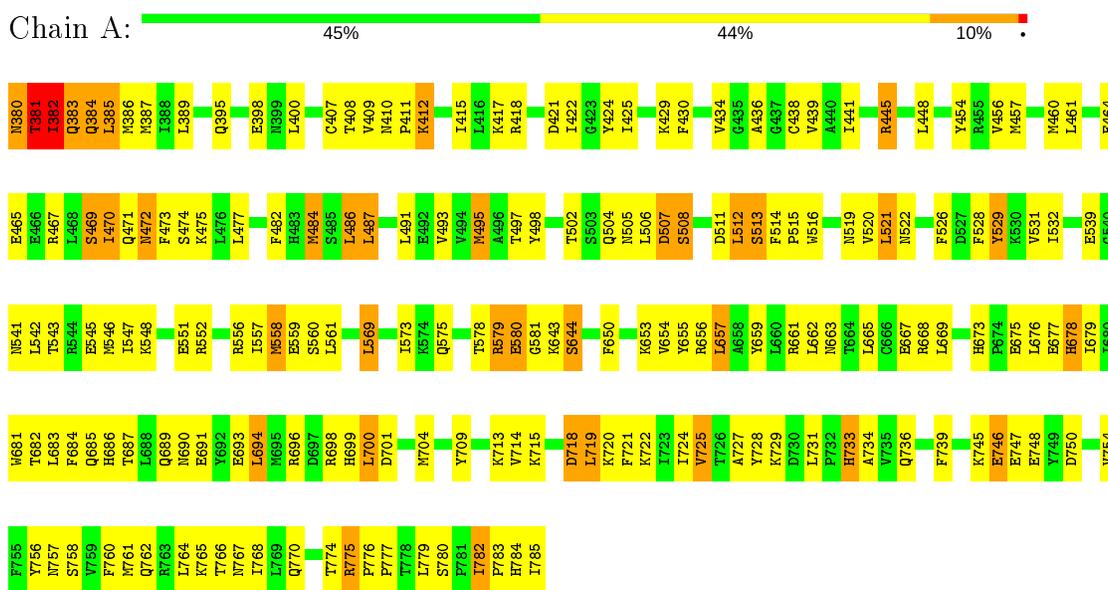
Chain A:

• Molecule 1: Retinoblastoma Pocket
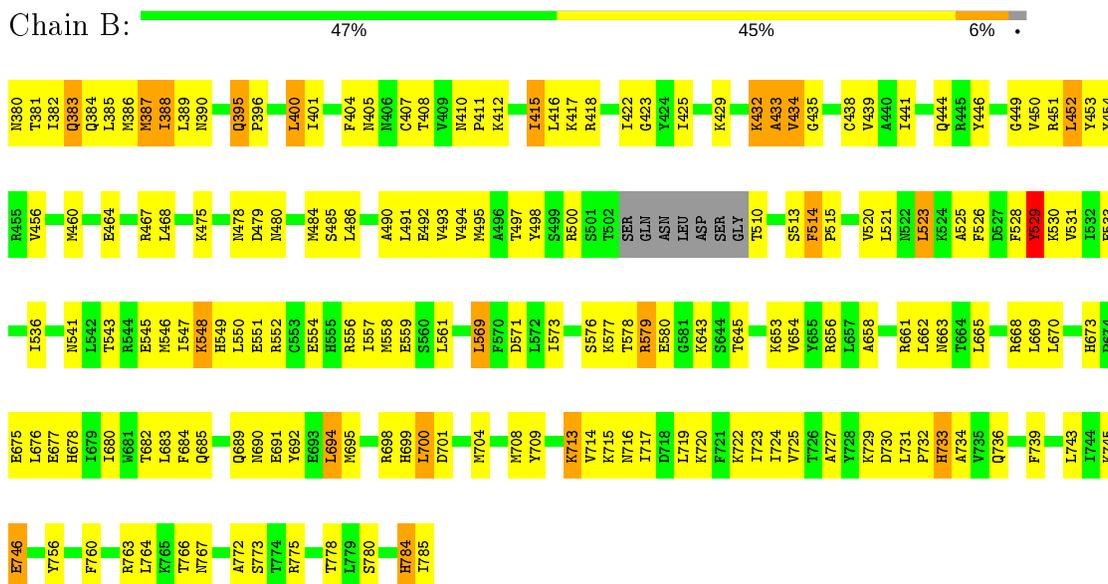
Chain B:

• Molecule 2: Transcription factor E2F2

Chain C:

• Molecule 2: Transcription factor E2F2

Chain D:

• Molecule 2: Transcription factor E2F2

Chain E:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.37Å 65.16Å 69.34Å 85.55° 79.48° 67.16°	Depositor
Resolution (Å)	19.65 – 2.20	Depositor
% Data completeness (in resolution range)	85.5 (19.65-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6249	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.48	0/2885	0.67	0/3887
1	B	0.46	0/2835	0.64	0/3818
2	C	0.50	0/146	0.70	0/196
2	D	0.39	0/146	0.58	0/196
2	E	0.63	0/95	1.13	1/128 (0.8%)
All	All	0.47	0/6107	0.67	1/8225 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	415	GLY	N-CA-C	-5.23	100.03	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	529	TYR	Sidechain

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	A	2829	0	2886	224	0
1	B	2780	0	2843	210	0
2	C	143	0	118	8	0
2	D	143	0	118	17	0
2	E	93	0	74	16	0
3	A	144	0	0	15	0
3	B	100	0	0	12	0
3	C	4	0	0	2	0
3	D	6	0	0	0	0
3	E	7	0	0	0	0
All	All	6249	0	6039	447	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 37.

The worst 5 of 447 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:385:LEU:HD13	1:B:388:ILE:HD11	1.33	1.08
1:A:774:THR:HG23	1:A:775:ARG:HD3	1.36	1.04
1:B:552:ARG:HH12	1:B:733:HIS:HB3	1.24	0.99
1:A:643:LYS:HG2	1:A:644:SER:H	1.28	0.99
1:B:694:LEU:HD13	1:B:763:ARG:HH21	1.26	0.98

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 X-ray entries followed by that with respect to entries of similar resolution.

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	343/345 (99%)	303 (88%)	23 (7%)	17 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	B	334/345 (97%)	301 (90%)	23 (7%)	10 (3%)	4	2	
2	C	16/18 (89%)	15 (94%)	0	1 (6%)	1	0	
2	D	16/18 (89%)	11 (69%)	3 (19%)	2 (12%)	0	0	
2	E	10/18 (56%)	5 (50%)	2 (20%)	3 (30%)	0	0	
All	All	719/744 (97%)	635 (88%)	51 (7%)	33 (5%)	2	1	

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	THR
1	A	382	ILE
1	A	507	ASP
1	A	513	SER
1	A	718	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	321/321 (100%)	287 (89%)	34 (11%)	6	6
1	B	315/321 (98%)	296 (94%)	19 (6%)	19	22
2	C	14/14 (100%)	14 (100%)	0	100	100
2	D	14/14 (100%)	14 (100%)	0	100	100
2	E	8/14 (57%)	4 (50%)	4 (50%)	0	0
All	All	672/684 (98%)	615 (92%)	57 (8%)	10	10

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	683	LEU
1	A	758	SER
1	B	778	THR
1	A	694	LEU

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Mol	Chain	Res	Type
1	A	721	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	767	ASN
1	B	383	GLN
1	B	733	HIS
1	B	380	ASN
1	B	395	GLN

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.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.