



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 08:39 am BST

PDB ID : 1O9K
Title : Crystal structure of the retinoblastoma tumour suppressor protein bound to E2F peptide
Authors : Xiao, B.; Spencer, J.; Clements, A.; Ali-Khan, N.; Mittnacht, S.; Broceno, C.; Burghammer, M.; Perrakis, A.; Marmorstein, R.; Gamblin, S.J.
Deposited on : 2002-12-16
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

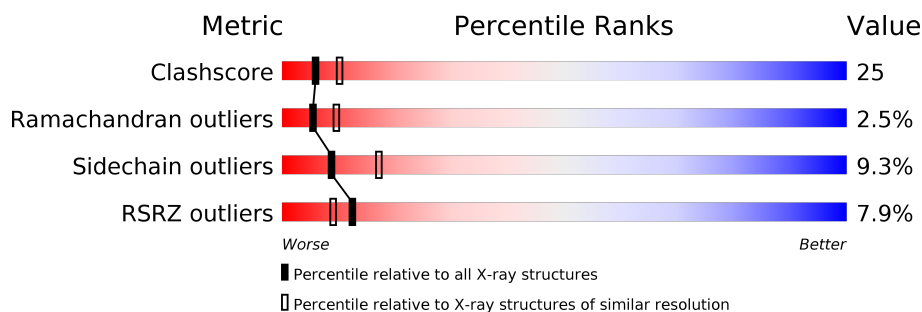
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div> <div>3%</div> <div>56%</div> <div>27%</div> <div>6%</div> <div>11%</div> </div>
1	C	218	<div> <div>4%</div> <div>57%</div> <div>25%</div> <div>6%</div> <div>11%</div> </div>
1	E	218	<div> <div>5%</div> <div>51%</div> <div>31%</div> <div>6%</div> <div>11%</div> </div>
1	G	218	<div> <div>5%</div> <div>51%</div> <div>32%</div> <div>6%</div> <div>11%</div> </div>
2	B	152	<div> <div>9%</div> <div>59%</div> <div>31%</div> <div>5%</div> <div>5%</div> </div>
2	D	152	<div> <div>8%</div> <div>57%</div> <div>34%</div> <div>5%</div> </div>
2	F	152	<div> <div>11%</div> <div>56%</div> <div>31%</div> <div>7%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	152	<div><div></div><div>9%</div><div>48%</div><div>41%</div><div>6%</div><div>5%</div></div>
3	P	18	<div><div></div><div>22%</div><div>67%</div><div>22%</div><div>11%</div></div>
3	Q	18	<div><div></div><div>22%</div><div>50%</div><div>33%</div><div>11%</div><div>6%</div></div>
3	R	18	<div><div></div><div>33%</div><div>39%</div><div>33%</div><div>22%</div><div>6%</div></div>
3	S	18	<div><div></div><div>28%</div><div>39%</div><div>44%</div><div>17%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11974 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-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	C	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	E	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	G	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			

- Molecule 2 is a protein called RETINOBLASTOMA-ASSOCIATED PROTEIN.

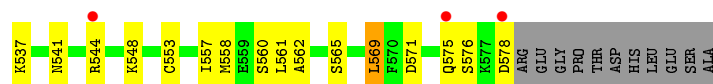
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	D	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	F	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	H	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			

- Molecule 3 is a protein called TRANSCRIPTION FACTOR E2F1.

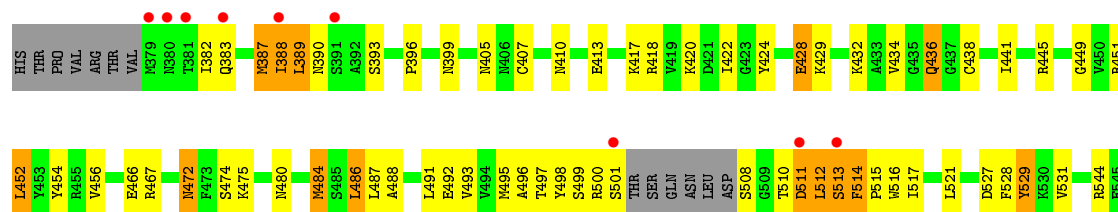
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	Q	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	R	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	S	18	Total	C	N	O	0	0	0
			149	96	23	30			

- Molecule 4 is water.

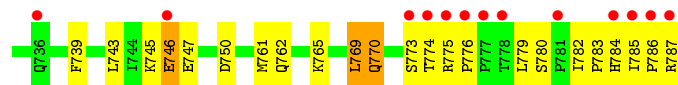
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total 39	O 39	0	0
4	B	18	Total 18	O 18	0	0
4	C	47	Total 47	O 47	0	0
4	D	24	Total 24	O 24	0	0
4	E	38	Total 38	O 38	0	0
4	F	16	Total 16	O 16	0	0
4	G	39	Total 39	O 39	0	0
4	H	15	Total 15	O 15	0	0
4	P	1	Total 1	O 1	0	0
4	Q	4	Total 4	O 4	0	0
4	R	4	Total 4	O 4	0	0
4	S	5	Total 5	O 5	0	0



• Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN



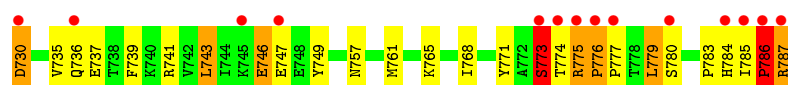
• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN



• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN

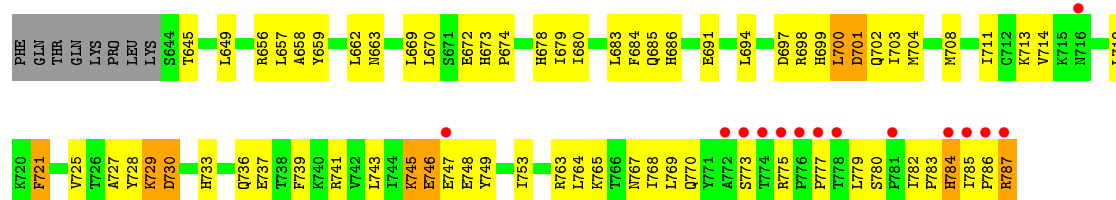


• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN



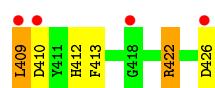
- Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN

Chain H: 



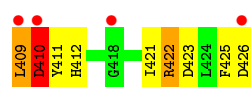
- Molecule 3: TRANSCRIPTION FACTOR E2F1

Chain P: 




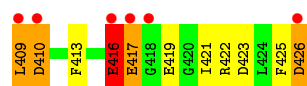
- Molecule 3: TRANSCRIPTION FACTOR E2F1

Chain Q: 



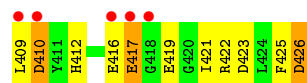
- Molecule 3: TRANSCRIPTION FACTOR E2F1

Chain R: 



- Molecule 3: TRANSCRIPTION FACTOR E2F1

Chain S: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.00Å 158.55Å 110.62Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.2 (20.00-2.60) 88.1 (19.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.229 , 0.285 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.55	0/1595	0.83	3/2141 (0.1%)
1	C	0.52	0/1595	0.81	5/2141 (0.2%)
1	E	0.52	0/1595	0.78	6/2141 (0.3%)
1	G	0.53	0/1595	0.77	5/2141 (0.2%)
2	B	0.46	0/1242	0.72	1/1680 (0.1%)
2	D	0.43	0/1242	0.72	2/1680 (0.1%)
2	F	0.39	0/1242	0.72	1/1680 (0.1%)
2	H	0.44	0/1242	0.73	3/1680 (0.2%)
3	P	0.47	0/152	0.91	1/203 (0.5%)
3	Q	0.40	0/152	0.83	1/203 (0.5%)
3	R	0.49	0/152	0.98	2/203 (1.0%)
3	S	0.42	0/152	0.87	1/203 (0.5%)
All	All	0.49	0/11956	0.77	31/16096 (0.2%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	GLY	N-CA-C	-9.23	90.02	113.10
1	A	571	ASP	CB-CG-OD2	6.71	124.34	118.30
1	C	468	LEU	N-CA-C	-6.58	93.24	111.00
2	H	730	ASP	CB-CG-OD2	6.32	123.99	118.30
2	H	701	ASP	CB-CG-OD2	6.17	123.85	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1569	0	1592	84	0
1	C	1569	0	1592	76	0
1	E	1569	0	1592	106	0
1	G	1569	0	1592	112	0
2	B	1213	0	1246	45	0
2	D	1213	0	1246	43	0
2	F	1213	0	1246	57	0
2	H	1213	0	1246	63	0
3	P	149	0	129	4	0
3	Q	149	0	129	11	0
3	R	149	0	129	17	0
3	S	149	0	129	10	0
4	A	39	0	0	9	0
4	B	18	0	0	3	0
4	C	47	0	0	14	0
4	D	24	0	0	1	0
4	E	38	0	0	8	0
4	F	16	0	0	3	0
4	G	39	0	0	9	0
4	H	15	0	0	8	0
4	P	1	0	0	0	0
4	Q	4	0	0	1	0
4	R	4	0	0	1	0
4	S	5	0	0	3	0
All	All	11974	0	11868	588	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 25.

The worst 5 of 588 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:A:512:LEU:HD22	1:A:512:LEU:O	1.28	1.27
1:C:513:SER:O	1:C:515:PRO:HD2	1.35	1.23
2:H:737:GLU:HB2	4:H:2008:HOH:O	1.36	1.21
1:C:509:GLY:HA2	4:C:2028:HOH:O	1.50	1.10
1:A:512:LEU:CD2	1:A:512:LEU:O	2.05	1.04

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	190/218 (87%)	178 (94%)	6 (3%)	6 (3%)	4	6
1	C	190/218 (87%)	170 (90%)	14 (7%)	6 (3%)	4	6
1	E	190/218 (87%)	178 (94%)	10 (5%)	2 (1%)	14	30
1	G	190/218 (87%)	174 (92%)	10 (5%)	6 (3%)	4	6
2	B	142/152 (93%)	129 (91%)	11 (8%)	2 (1%)	11	22
2	D	142/152 (93%)	127 (89%)	13 (9%)	2 (1%)	11	22
2	F	142/152 (93%)	127 (89%)	11 (8%)	4 (3%)	5	7
2	H	142/152 (93%)	124 (87%)	15 (11%)	3 (2%)	7	13
3	P	16/18 (89%)	14 (88%)	2 (12%)	0	100	100
3	Q	16/18 (89%)	14 (88%)	1 (6%)	1 (6%)	1	1
3	R	16/18 (89%)	13 (81%)	1 (6%)	2 (12%)	0	0
3	S	16/18 (89%)	13 (81%)	2 (12%)	1 (6%)	1	1
All	All	1392/1552 (90%)	1261 (91%)	96 (7%)	35 (2%)	5	9

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PHE
1	C	514	PHE
2	D	784	HIS
2	D	786	PRO
2	F	779	LEU

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	178/200 (89%)	162 (91%)	16 (9%)	9	18
1	C	178/200 (89%)	163 (92%)	15 (8%)	11	21
1	E	178/200 (89%)	160 (90%)	18 (10%)	7	14
1	G	178/200 (89%)	163 (92%)	15 (8%)	11	21
2	B	139/147 (95%)	123 (88%)	16 (12%)	5	10
2	D	139/147 (95%)	127 (91%)	12 (9%)	10	20
2	F	139/147 (95%)	126 (91%)	13 (9%)	8	17
2	H	139/147 (95%)	129 (93%)	10 (7%)	14	29
3	P	15/15 (100%)	13 (87%)	2 (13%)	4	7
3	Q	15/15 (100%)	13 (87%)	2 (13%)	4	7
3	R	15/15 (100%)	11 (73%)	4 (27%)	0	1
3	S	15/15 (100%)	14 (93%)	1 (7%)	16	33
All	All	1328/1448 (92%)	1204 (91%)	124 (9%)	9	17

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	746	GLU
1	E	486	LEU
2	H	787	ARG
2	D	750	ASP
1	E	413	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	555	HIS
1	E	436	GLN
2	H	689	GLN
2	D	689	GLN
1	E	383	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	194/218 (88%)	0.01	6 (3%) 49 42	20, 29, 56, 74	0
1	C	194/218 (88%)	-0.02	9 (4%) 32 26	20, 29, 55, 69	0
1	E	194/218 (88%)	0.16	11 (5%) 23 18	21, 30, 57, 77	0
1	G	194/218 (88%)	0.07	11 (5%) 23 18	21, 29, 58, 75	0
2	B	144/152 (94%)	0.37	14 (9%) 7 5	21, 38, 71, 79	0
2	D	144/152 (94%)	0.43	12 (8%) 11 8	24, 39, 72, 80	0
2	F	144/152 (94%)	0.56	17 (11%) 4 3	27, 43, 73, 80	0
2	H	144/152 (94%)	0.51	14 (9%) 7 5	27, 40, 72, 83	0
3	P	18/18 (100%)	0.83	4 (22%) 0 0	41, 48, 61, 64	0
3	Q	18/18 (100%)	0.80	4 (22%) 0 0	40, 49, 58, 61	0
3	R	18/18 (100%)	1.09	6 (33%) 0 0	39, 52, 65, 68	0
3	S	18/18 (100%)	1.17	5 (27%) 0 0	41, 51, 62, 64	0
All	All	1424/1552 (91%)	0.27	113 (7%) 12 9	20, 36, 65, 83	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	774	THR	9.1
2	D	774	THR	8.8
1	E	379	MET	7.6
2	B	776	PRO	7.2
2	H	787	ARG	7.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.