



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 06:17 AM EST

PDB ID : 4ELL
Title : Structure of the inactive retinoblastoma protein pocket domain
Authors : Burke, J.R.; Rubin, S.M.
Deposited on : 2012-04-10
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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) : 2.36

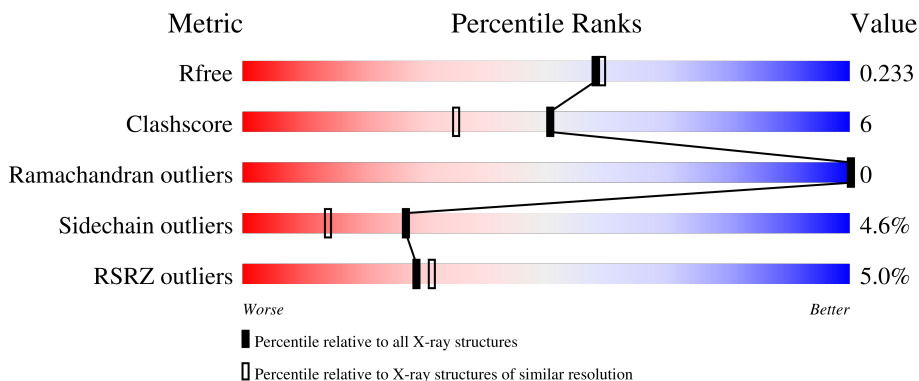
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 of 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	411	 8% 68% 12% 19%
1	B	411	 71% 14% 15%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5961 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
			Total	C	N	O	S			
1	A	331	2733	1768	453	492	20	0	0	0
1	B	349	2873	1852	479	521	21	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	GLY	-	expression tag	UNP P06400
A	378	GLU	-	expression tag	UNP P06400
A	379	PHE	-	expression tag	UNP P06400
A	561	PHE	LEU	engineered mutation	UNP P06400
A	608	GLU	SER	engineered mutation	UNP P06400
A	612	ALA	SER	conflict	UNP P06400
A	780	ALA	SER	conflict	UNP P06400
B	377	GLY	-	expression tag	UNP P06400
B	378	GLU	-	expression tag	UNP P06400
B	379	PHE	-	expression tag	UNP P06400
B	561	PHE	LEU	engineered mutation	UNP P06400
B	608	GLU	SER	engineered mutation	UNP P06400
B	612	ALA	SER	conflict	UNP P06400
B	780	ALA	SER	conflict	UNP P06400

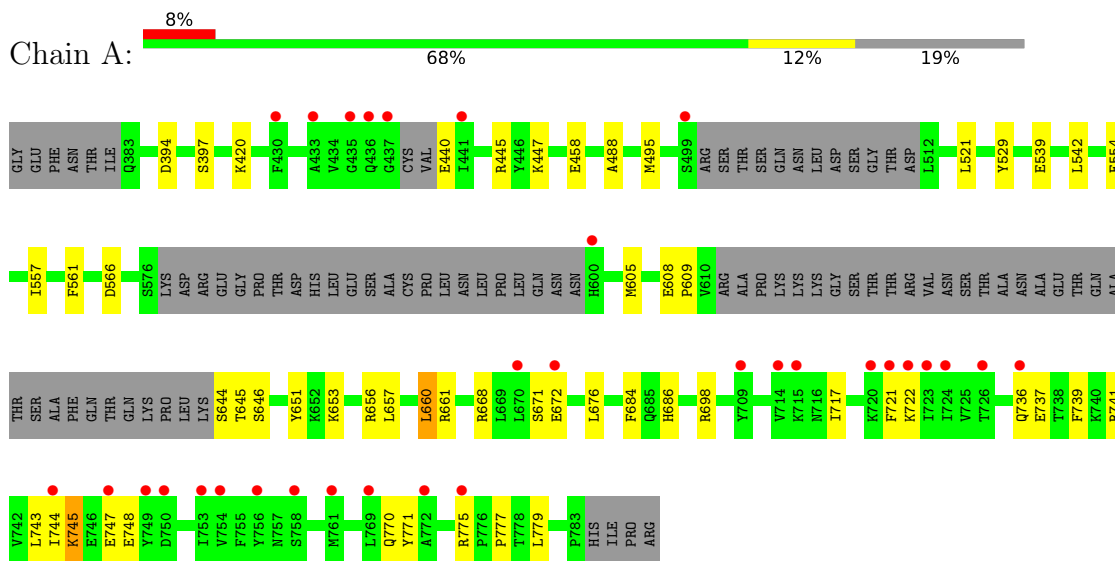
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total 99	O 99	0	0
2	B	256	Total 256	O 256	0	0

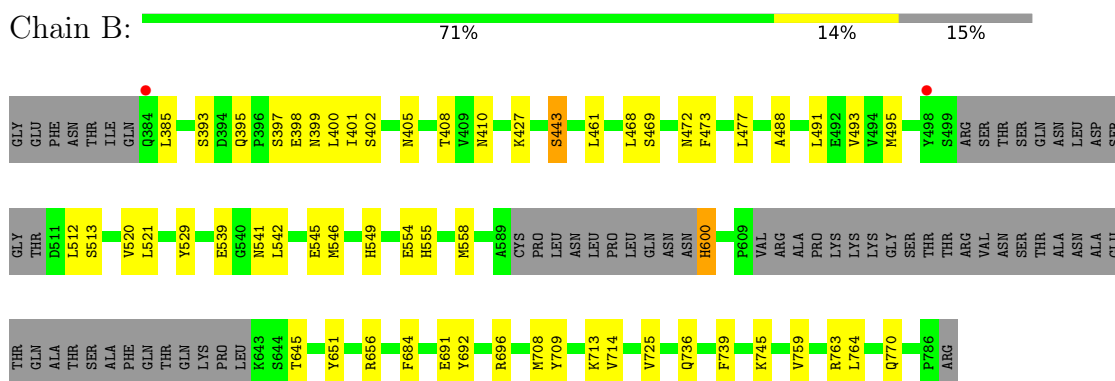
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Retinoblastoma-associated protein



- Molecule 1: Retinoblastoma-associated protein



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	249.66Å 249.66Å 35.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.03 – 1.98 36.04 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.03-1.98) 99.9 (36.04-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.98Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.193 , 0.238 0.189 , 0.233	Depositor DCC
R_{free} test set	1993 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5961	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.36	0/2788	0.48	0/3754
1	B	0.49	0/2933	0.54	0/3952
All	All	0.43	0/5721	0.51	0/7706

There are no bond length outliers.

There are no bond angle outliers.

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	2733	0	2774	31	0
1	B	2873	0	2905	34	0
2	A	99	0	0	6	0
2	B	256	0	0	7	0
All	All	5961	0	5679	64	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 6.

All (64) 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:600:HIS:HD1	1:B:600:HIS:N	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:GLU:HG2	1:B:558:MET:HE2	1.63	0.80
1:B:600:HIS:N	1:B:600:HIS:ND1	2.30	0.79
1:A:775:ARG:NH2	1:B:513:SER:OG	2.21	0.74
1:A:770:GLN:OE1	2:A:819:HOH:O	2.08	0.71
1:B:696:ARG:NH1	2:B:865:HOH:O	1.97	0.70
1:B:645:THR:HG23	2:B:1027:HOH:O	1.91	0.70
1:B:656:ARG:NH1	2:B:830:HOH:O	2.06	0.69
1:B:692:TYR:OH	2:B:1045:HOH:O	2.11	0.66
1:A:698:ARG:NH1	1:A:743:LEU:O	2.31	0.64
1:B:770:GLN:NE2	2:B:975:HOH:O	2.34	0.61
1:B:405:ASN:HD22	1:B:410:ASN:HD21	1.48	0.61
1:A:554:GLU:OE2	1:A:653:LYS:NZ	2.36	0.59
1:A:557:ILE:HA	1:A:561:PHE:HB2	1.84	0.59
1:B:399:ASN:O	1:B:402:SER:OG	2.18	0.58
1:B:427:LYS:HD3	1:B:443:SER:HB3	1.85	0.58
1:A:657:LEU:HD21	1:A:661:ARG:CZ	2.35	0.57
1:A:566:ASP:OD1	2:A:873:HOH:O	2.18	0.56
1:B:554:GLU:HG2	1:B:558:MET:CE	2.36	0.56
1:A:445:ARG:HD2	1:A:495:MET:HE1	1.88	0.54
1:A:660:LEU:HG	1:A:661:ARG:N	2.22	0.54
1:B:493:VAL:HG13	1:B:546:MET:HG2	1.89	0.54
1:A:605:MET:CE	1:A:646:SER:HA	2.38	0.53
1:B:546:MET:HE3	1:B:549:HIS:HB3	1.92	0.51
1:B:488:ALA:HB2	1:B:521:LEU:HD12	1.93	0.51
1:B:709:TYR:OH	1:B:713:LYS:HE2	2.11	0.50
1:A:744:ILE:HG22	1:A:745:LYS:HD3	1.93	0.49
1:A:747:GLU:O	1:A:747:GLU:HG3	2.12	0.49
1:B:491:LEU:O	1:B:495:MET:HG2	2.12	0.49
1:A:745:LYS:O	1:A:748:GLU:HG2	2.14	0.48
1:B:555:HIS:HD2	1:B:558:MET:HE3	1.76	0.48
1:A:653:LYS:HE3	2:A:818:HOH:O	2.14	0.48
1:A:394:ASP:OD1	1:A:447:LYS:HE2	2.14	0.48
1:A:676:LEU:HD11	1:A:717:ILE:HD13	1.97	0.47
1:A:539:GLU:HG3	1:A:542:LEU:HG	1.97	0.46
1:B:472:ASN:HA	2:B:1044:HOH:O	2.15	0.46
1:A:736:GLN:HA	1:A:739:PHE:CE2	2.49	0.46
1:A:488:ALA:HB2	1:A:521:LEU:HD12	1.98	0.46
1:A:605:MET:HE2	1:A:646:SER:HA	1.98	0.46
1:A:420:LYS:HD3	2:A:883:HOH:O	2.15	0.45
1:A:771:TYR:CE1	1:A:777:PRO:HG2	2.50	0.45
1:A:397:SER:OG	1:A:458:GLU:OE2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ARG:HB3	1:A:495:MET:HE3	1.99	0.44
1:B:545:GLU:CD	2:B:860:HOH:O	2.55	0.44
1:A:440:GLU:N	2:A:842:HOH:O	2.51	0.43
1:B:469:SER:H	1:B:472:ASN:HD22	1.66	0.43
1:A:445:ARG:HB3	1:A:495:MET:CE	2.48	0.43
1:B:397:SER:O	1:B:401:ILE:HG12	2.18	0.43
1:A:653:LYS:HG3	1:A:656:ARG:HH21	1.83	0.43
1:B:555:HIS:HD2	1:B:558:MET:CE	2.30	0.43
1:B:493:VAL:HG22	1:B:546:MET:HE2	2.01	0.42
1:B:691:GLU:HG3	1:B:764:LEU:HD21	2.01	0.42
1:B:461:LEU:HD11	1:B:477:LEU:HD21	2.01	0.42
1:A:608:GLU:HA	1:A:609:PRO:HD3	1.91	0.42
1:B:736:GLN:HA	1:B:739:PHE:CE2	2.54	0.42
1:A:737:GLU:HG2	1:A:741:ARG:HE	1.84	0.42
1:B:468:LEU:HB3	1:B:472:ASN:HB2	2.02	0.42
1:B:385:LEU:HB2	1:B:541:ASN:HB3	2.01	0.42
1:B:555:HIS:HA	1:B:558:MET:HE3	2.02	0.42
1:A:644:SER:N	2:A:843:HOH:O	2.52	0.42
1:B:745:LYS:HE3	1:B:759:VAL:HG22	2.02	0.42
1:A:605:MET:HE3	1:A:646:SER:HA	2.03	0.41
1:B:520:VAL:HG12	1:B:521:LEU:HD23	2.03	0.41
1:B:539:GLU:HG3	1:B:542:LEU:HG	2.04	0.40

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	321/411 (78%)	313 (98%)	8 (2%)	0	100	100
1	B	341/411 (83%)	338 (99%)	3 (1%)	0	100	100
All	All	662/822 (80%)	651 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	308/378 (82%)	295 (96%)	13 (4%)	30	17
1	B	324/378 (86%)	308 (95%)	16 (5%)	25	12
All	All	632/756 (84%)	603 (95%)	29 (5%)	27	14

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	529	TYR
1	A	645	THR
1	A	651	TYR
1	A	660	LEU
1	A	668	ARG
1	A	671	SER
1	A	672	GLU
1	A	684	PHE
1	A	686	HIS
1	A	721	PHE
1	A	722	LYS
1	A	745	LYS
1	A	779	LEU
1	B	393	SER
1	B	395	GLN
1	B	398	GLU
1	B	400	LEU
1	B	408	THR
1	B	443	SER
1	B	473	PHE
1	B	512	LEU
1	B	529	TYR
1	B	600	HIS
1	B	651	TYR
1	B	684	PHE

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Mol	Chain	Res	Type
1	B	708	MET
1	B	714	VAL
1	B	725	VAL
1	B	763	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	405	ASN
1	B	472	ASN
1	B	555	HIS

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 monosaccharides 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

6.1 Protein, DNA and RNA chains

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	331/411 (80%)	0.39	32 (9%) 7 8	26, 46, 67, 85	0
1	B	349/411 (84%)	0.04	2 (0%) 89 90	13, 29, 56, 67	0
All	All	680/822 (82%)	0.21	34 (5%) 28 31	13, 39, 64, 85	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436	GLN	6.1
1	A	721	PHE	3.8
1	A	769	LEU	3.8
1	A	435	GLY	3.7
1	A	441	ILE	3.5
1	A	437	GLY	3.4
1	A	714	VAL	3.1
1	A	754	VAL	3.1
1	A	720	LYS	3.1
1	A	722	LYS	3.0
1	A	600	HIS	3.0
1	A	499	SER	3.0
1	A	726	THR	2.9
1	A	753	ILE	2.9
1	A	724	ILE	2.8
1	A	761	MET	2.7
1	A	756	TYR	2.6
1	A	747	GLU	2.6
1	A	758	SER	2.5
1	A	723	ILE	2.4
1	A	430	PHE	2.4
1	B	498	TYR	2.4
1	A	736	GLN	2.2
1	B	384	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	670	LEU	2.2
1	A	775	ARG	2.1
1	A	749	TYR	2.1
1	A	672	GLU	2.1
1	A	709	TYR	2.1
1	A	750	ASP	2.1
1	A	744	ILE	2.1
1	A	433	ALA	2.0
1	A	715	LYS	2.0
1	A	772	ALA	2.0

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 monosaccharides 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.