



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 09:23 am GMT

PDB ID : 2WB0
Title : 2.1 resolution structure of the C-terminal domain of the human adenovirus 5 ssDNA binding protein
Authors : Hendle, J.; Kanellopoulos, P.N.; Tucker, P.A.
Deposited on : 2009-02-19
Resolution : 1.95 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

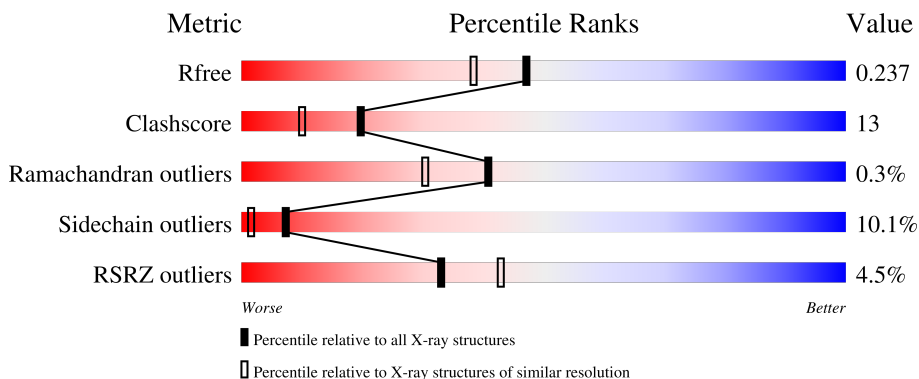
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	X	356	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2862 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 E2A DNA-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	314	2477	1574	432	448	23	0	1	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	2	Total	Zn	0	0
			2	2		

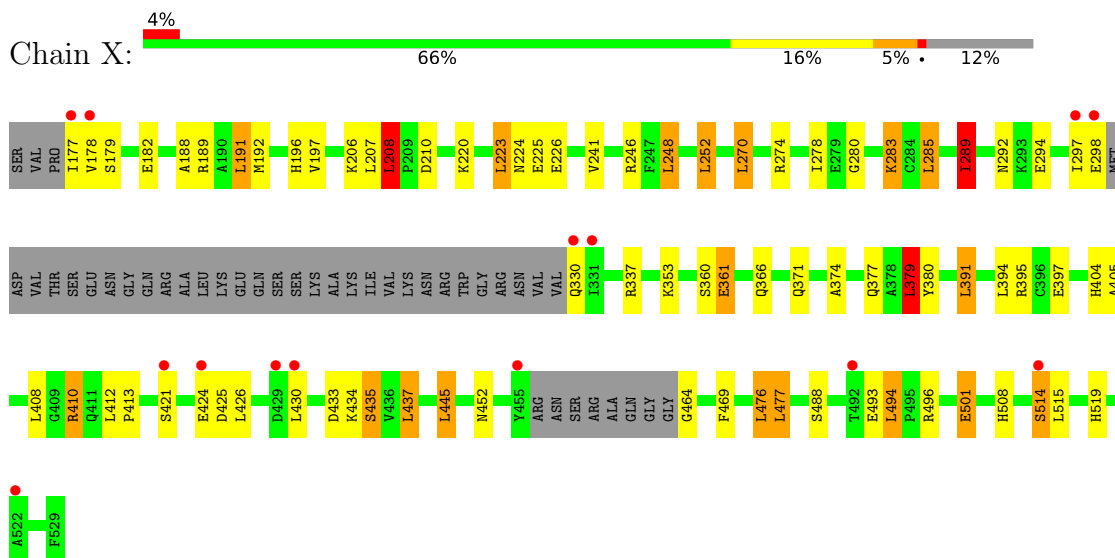
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	383	Total	O	0	0
			383	383		

3 Residue-property plots

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: E2A DNA-BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.29Å 76.66Å 64.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.95 – 1.95 14.95 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (14.95-1.95) 98.4 (14.95-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.184 , 0.245 0.189 , 0.237	Depositor DCC
R_{free} test set	1436 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.013 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2862	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	X	1.12	5/2540 (0.2%)	1.09	23/3438 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	501	GLU	CD-OE1	9.04	1.35	1.25
1	X	435	SER	CB-OG	-6.27	1.34	1.42
1	X	283	LYS	CE-NZ	5.62	1.63	1.49
1	X	514	SER	CB-OG	5.41	1.49	1.42
1	X	469	PHE	CE1-CZ	5.36	1.47	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	337	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	X	379	LEU	CA-CB-CG	8.49	134.83	115.30
1	X	270	LEU	CB-CG-CD1	7.61	123.94	111.00
1	X	391	LEU	CB-CG-CD2	7.33	123.47	111.00
1	X	191	LEU	CB-CG-CD1	7.28	123.38	111.00
1	X	476	LEU	CB-CG-CD2	7.22	123.28	111.00
1	X	410	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	X	283	LYS	CD-CE-NZ	6.74	127.20	111.70
1	X	223	LEU	CB-CG-CD1	6.26	121.65	111.00
1	X	252	LEU	CA-CB-CG	6.21	129.60	115.30
1	X	210	ASP	CB-CG-OD1	6.13	123.82	118.30
1	X	248	LEU	CB-CG-CD2	6.06	121.31	111.00
1	X	337	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	X	437	LEU	CB-CG-CD1	5.87	120.98	111.00
1	X	494	LEU	CA-CB-CG	5.69	128.39	115.30
1	X	285	LEU	CB-CG-CD1	5.59	120.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	477	LEU	CB-CG-CD2	5.56	120.45	111.00
1	X	445	LEU	CB-CG-CD1	5.51	120.37	111.00
1	X	395	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	X	208	LEU	CB-CG-CD1	5.46	120.28	111.00
1	X	289	ILE	CB-CG1-CD1	-5.37	98.86	113.90
1	X	289	ILE	CA-CB-CG2	5.29	121.48	110.90
1	X	252	LEU	CB-CG-CD1	5.09	119.65	111.00

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	X	2477	0	2415	62	0
2	X	2	0	0	0	0
3	X	383	0	0	39	1
All	All	2862	0	2415	62	1

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 13.

All (62) 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:X:178:VAL:HG23	3:X:2005:HOH:O	1.19	1.34
1:X:397:GLU:HB3	3:X:2246:HOH:O	1.44	1.17
1:X:412:LEU:HB2	3:X:2267:HOH:O	1.56	1.02
1:X:177:ILE:HG13	3:X:2001:HOH:O	1.59	1.00
1:X:246:ARG:HG2	3:X:2088:HOH:O	1.64	0.95
1:X:412:LEU:HD12	3:X:2267:HOH:O	1.68	0.93
1:X:410:ARG:H	1:X:452:ASN:HD21	1.21	0.86
1:X:178:VAL:HG13	3:X:2011:HOH:O	1.78	0.81
1:X:289:ILE:HD11	3:X:2158:HOH:O	1.80	0.81
1:X:394:LEU:HD22	1:X:412:LEU:HD22	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:280:GLY:H	1:X:366:GLN:HE22	1.32	0.76
1:X:178:VAL:CG2	3:X:2005:HOH:O	1.96	0.74
1:X:519:HIS:CD2	3:X:2368:HOH:O	2.42	0.71
1:X:182:GLU:OE1	3:X:2011:HOH:O	2.09	0.71
1:X:434:LYS:HE2	3:X:2274:HOH:O	1.91	0.70
1:X:434:LYS:HE3	3:X:2279:HOH:O	1.90	0.70
1:X:394:LEU:CD2	1:X:412:LEU:HD22	2.21	0.70
1:X:433:ASP:OD1	1:X:435:SER:HB2	1.92	0.70
1:X:514:SER:HA	3:X:2362:HOH:O	1.91	0.69
1:X:488:SER:HB3	3:X:2319:HOH:O	1.93	0.68
1:X:519:HIS:NE2	3:X:2368:HOH:O	2.27	0.68
1:X:182:GLU:OE2	3:X:2010:HOH:O	2.12	0.67
1:X:412:LEU:CD1	3:X:2267:HOH:O	2.35	0.66
1:X:412:LEU:CB	3:X:2267:HOH:O	2.27	0.66
1:X:394:LEU:HD22	1:X:412:LEU:CD2	2.26	0.63
1:X:177:ILE:N	3:X:2001:HOH:O	2.32	0.62
1:X:220:LYS:HD3	1:X:241:VAL:HG21	1.81	0.61
1:X:179:SER:N	3:X:2011:HOH:O	2.33	0.58
1:X:224:ASN:HB3	3:X:2060:HOH:O	2.04	0.57
1:X:410:ARG:N	1:X:452:ASN:HD21	1.99	0.55
1:X:292:ASN:HB3	3:X:2171:HOH:O	2.07	0.55
1:X:353:LYS:HE3	3:X:2199:HOH:O	2.07	0.54
1:X:424:GLU:C	1:X:426:LEU:H	2.11	0.53
1:X:496:ARG:NH2	3:X:2334:HOH:O	2.39	0.53
1:X:374:ALA:HA	1:X:377:GLN:HE21	1.74	0.53
1:X:496:ARG:NE	3:X:2334:HOH:O	2.30	0.52
1:X:246:ARG:CD	3:X:2088:HOH:O	2.59	0.51
1:X:177:ILE:HG23	3:X:2004:HOH:O	2.11	0.51
1:X:412:LEU:CG	3:X:2267:HOH:O	2.52	0.50
1:X:280:GLY:H	1:X:366:GLN:NE2	2.06	0.50
1:X:274:ARG:HB2	1:X:283:LYS:HD2	1.94	0.49
1:X:404:HIS:HD2	1:X:405:ALA:O	1.94	0.48
1:X:189:ARG:NH2	3:X:2017:HOH:O	2.41	0.48
1:X:412:LEU:HD11	1:X:508:HIS:HB3	1.95	0.47
1:X:177:ILE:HG22	3:X:2003:HOH:O	2.14	0.47
1:X:246:ARG:CG	3:X:2088:HOH:O	2.38	0.47
1:X:206:LYS:HB2	1:X:208:LEU:HD22	1.96	0.46
1:X:220:LYS:NZ	3:X:2053:HOH:O	2.48	0.46
1:X:189:ARG:HA	1:X:189:ARG:HD3	1.89	0.45
1:X:361:GLU:HB2	3:X:2212:HOH:O	2.16	0.44
1:X:192:MET:HA	1:X:197:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:434:LYS:CE	3:X:2274:HOH:O	2.59	0.44
1:X:298:GLU:OE2	1:X:330:GLN:NE2	2.41	0.43
1:X:196:HIS:HB2	3:X:2024:HOH:O	2.18	0.43
1:X:464:GLY:N	3:X:2301:HOH:O	2.52	0.43
1:X:294:GLU:HB3	3:X:2162:HOH:O	2.20	0.42
1:X:188:ALA:O	1:X:192:MET:HG3	2.19	0.42
1:X:379:LEU:HG	1:X:380:TYR:CE2	2.54	0.42
1:X:177:ILE:CG2	3:X:2003:HOH:O	2.68	0.41
1:X:412:LEU:HD21	1:X:508:HIS:ND1	2.36	0.41
1:X:297:ILE:HG22	1:X:298:GLU:N	2.36	0.40
1:X:225:GLU:HG2	1:X:226:GLU:HG2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:2065:HOH:O	3:X:2366:HOH:O[3_644]	2.15	0.05

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	X	309/356 (87%)	300 (97%)	7 (2%)	2 (1%)	25 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	421[A]	SER
1	X	421[B]	SER

5.3.2 Protein sidechains

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	X	269/303 (89%)	242 (90%)	27 (10%)	7 2

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	191	LEU
1	X	207	LEU
1	X	208	LEU
1	X	223	LEU
1	X	248	LEU
1	X	252	LEU
1	X	270	LEU
1	X	278	ILE
1	X	285	LEU
1	X	289	ILE
1	X	360	SER
1	X	361	GLU
1	X	371	GLN
1	X	379	LEU
1	X	391	LEU
1	X	408	LEU
1	X	413	PRO
1	X	425	ASP
1	X	430	LEU
1	X	437	LEU
1	X	445	LEU
1	X	476	LEU
1	X	477	LEU
1	X	493	GLU
1	X	494	LEU
1	X	501	GLU
1	X	515	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	204	ASN
1	X	224	ASN
1	X	249	GLN
1	X	292	ASN
1	X	366	GLN
1	X	371	GLN
1	X	404	HIS
1	X	452	ASN
1	X	490	ASN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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](#)

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	X	314/356 (88%)	0.10	14 (4%) 33 43	10, 22, 41, 57	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	455	TYR	7.3
1	X	178	VAL	4.5
1	X	430	LEU	4.0
1	X	177	ILE	3.9
1	X	331	ILE	3.4
1	X	298	GLU	3.0
1	X	429	ASP	2.8
1	X	297	ILE	2.8
1	X	421[A]	SER	2.8
1	X	330	GLN	2.7
1	X	492	THR	2.5
1	X	514	SER	2.4
1	X	522	ALA	2.4
1	X	424	GLU	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	X	601	1/1	1.00	0.06	16,16,16,16	0
2	ZN	X	602	1/1	1.00	0.05	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.