



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:36 AM UTC

PDB ID : 6BOW / pdb_00006bow
Title : Human APE1 substrate complex with an T/T mismatch adjacent the THF
Authors : Freudenthal, B.D.; Whitaker, A.M.; Fairlamb, M.S.
Deposited on : 2017-11-20
Resolution : 1.59 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

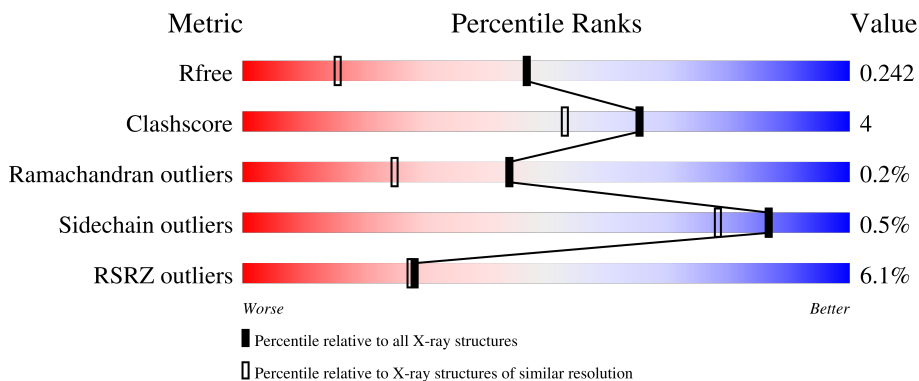
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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 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	318	
1	B	318	
2	P	21	
3	V	21	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5579 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 DNA-(apurinic or apyrimidinic site) lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	Total	C	N	O	S	0	3	0
			2100	1350	361	381	8			
1	B	268	Total	C	N	O	S	0	1	0
			2099	1351	360	380	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	ALA	CYS	engineered mutation	UNP P27695
B	138	ALA	CYS	engineered mutation	UNP P27695

- Molecule 2 is a DNA chain called 21-mer DNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	P	21	Total	C	N	O	P	S	0	1	0
			430	204	76	127	21	2			

- Molecule 3 is a DNA chain called 21-mer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	V	21	Total	C	N	O	P	0	0	0
			426	203	79	124	20			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	269	Total	O	0	0
			269	269		
4	B	156	Total	O	0	0
			156	156		
4	P	51	Total	O	0	0
			51	51		

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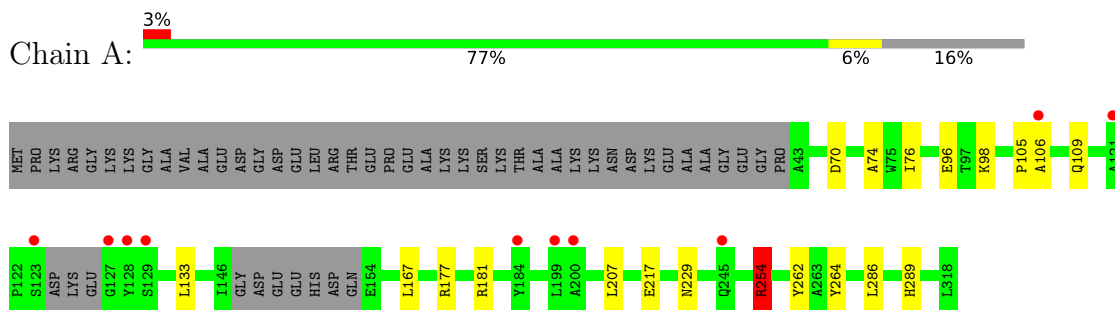
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	V	48	Total	O	0	0
			48	48		

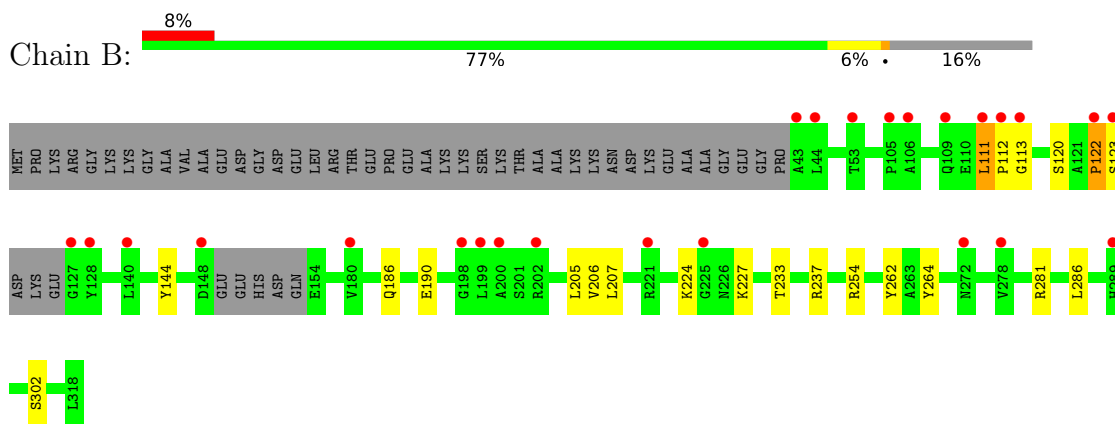
3 Residue-property plots [i](#)

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.

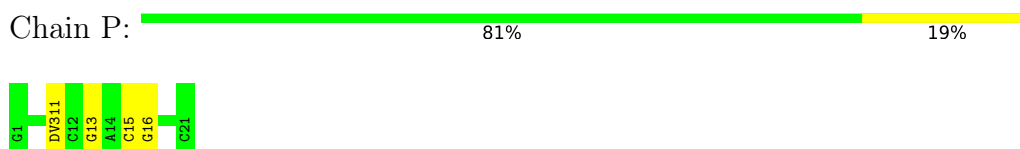
- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase



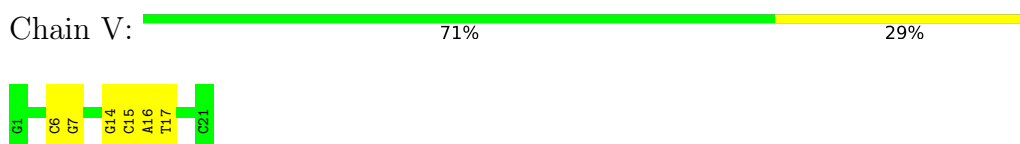
- Molecule 1: DNA-(apurinic or apyrimidinic site) lyase



- Molecule 2: 21-mer DNA



- Molecule 3: 21-mer DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.26Å 61.33Å 73.12Å 83.31° 78.28° 86.96°	Depositor
Resolution (Å)	24.56 – 1.59 24.56 – 1.59	Depositor EDS
% Data completeness (in resolution range)	95.0 (24.56-1.59) 80.6 (24.56-1.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 1.59Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.214 , 0.241 0.216 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtrriage
Anisotropy	0.377	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5579	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: DV3

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	0.64	2/2163 (0.1%)	0.72	0/2936
1	B	0.62	2/2158 (0.1%)	0.77	4/2930 (0.1%)
2	P	0.51	0/456	0.64	0/700
3	V	0.53	0/477	0.71	0/734
All	All	0.61	4/5254 (0.1%)	0.73	4/7300 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	GLY	C-N	-8.02	1.23	1.33
1	A	181	ARG	C-O	-5.17	1.17	1.24
1	B	111	LEU	C-N	5.13	1.39	1.34
1	A	254	ARG	C-O	-5.00	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	PRO	N-CA-C	7.31	123.14	113.57
1	B	111	LEU	CA-C-N	-6.30	113.31	119.87
1	B	111	LEU	C-N-CA	-6.30	113.31	119.87
1	B	112	PRO	N-CA-C	-5.26	107.56	114.03

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	2100	0	2088	16	0
1	B	2099	0	2065	10	0
2	P	430	0	226	6	0
3	V	426	0	237	5	0
4	A	269	0	0	6	0
4	B	156	0	0	1	0
4	P	51	0	0	5	0
4	V	48	0	0	0	0
All	All	5579	0	4616	35	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 4.

All (35) 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)
2:P:11[A]:DV3:SP3	4:P:124:HOH:O	2.33	0.87
2:P:11[A]:DV3:SP3	4:P:101:HOH:O	2.38	0.81
2:P:13:DG:N7	4:P:102:HOH:O	2.22	0.71
2:P:11[B]:DV3:OP2	4:P:101:HOH:O	2.10	0.69
1:A:229:ASN:HB2	4:A:406:HOH:O	1.93	0.69
1:A:289:HIS:ND1	4:A:401:HOH:O	2.29	0.65
1:A:177:ARG:NH1	4:A:403:HOH:O	2.33	0.61
2:P:13:DG:N3	4:P:103:HOH:O	2.30	0.59
1:A:96:GLU:OE1	1:A:98:LYS:HE2	2.02	0.59
1:A:106:ALA:HA	1:A:109:GLN:OE1	2.05	0.57
1:A:207:LEU:HD23	1:A:286:LEU:HD12	1.89	0.55
1:A:177:ARG:NH2	4:A:404:HOH:O	2.34	0.54
1:B:122:PRO:O	1:B:123:SER:OG	2.17	0.52
3:V:16:DA:H2''	3:V:17:DT:H5'	1.91	0.52
1:B:254:ARG:HG3	4:B:441:HOH:O	2.10	0.51
2:P:15:DC:H2''	2:P:16:DG:C8	2.49	0.48
1:B:186:GLN:O	1:B:190:GLU:HG3	2.14	0.47
3:V:6:DC:H2''	3:V:7:DG:C8	2.50	0.47
1:A:74:ALA:HB2	3:V:14:DG:H3'	1.97	0.46
1:A:98:LYS:HD3	3:V:15:DC:H5'	1.97	0.46
1:A:254:ARG:HA	1:A:254:ARG:HD3	1.56	0.46
1:B:207:LEU:HD23	1:B:286:LEU:HD12	1.99	0.45
3:V:16:DA:H2''	3:V:17:DT:C5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LYS:HA	1:B:227:LYS:HE3	1.98	0.44
1:B:254:ARG:HG2	1:B:281:ARG:NH1	2.33	0.44
1:A:262:TYR:HA	1:A:264:TYR:CZ	2.53	0.44
1:A:76:ILE:HD12	1:A:105:PRO:HG2	2.00	0.43
1:A:133:LEU:HD11	1:A:167:LEU:HD23	1.99	0.43
1:B:262:TYR:HA	1:B:264:TYR:CZ	2.54	0.42
1:A:70:ASP:HB2	4:A:537:HOH:O	2.20	0.42
1:B:120:SER:HB2	1:B:144:TYR:HD2	1.86	0.41
1:A:109:GLN:N	1:A:109:GLN:CD	2.78	0.41
1:B:205:LEU:HD23	1:B:206:VAL:C	2.45	0.41
1:B:233:THR:O	1:B:237:ARG:HG3	2.21	0.41
1:A:217:GLU:HG3	4:A:513:HOH:O	2.21	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	263/318 (83%)	260 (99%)	3 (1%)	0	100	100
1	B	263/318 (83%)	252 (96%)	10 (4%)	1 (0%)	30	14
All	All	526/636 (83%)	512 (97%)	13 (2%)	1 (0%)	44	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	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	224/265 (84%)	223 (100%)	1 (0%)	89	82
1	B	220/265 (83%)	219 (100%)	1 (0%)	86	78
All	All	444/530 (84%)	442 (100%)	2 (0%)	86	78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	ARG
1	B	302	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	117	GLN
1	B	186	GLN
1	B	255	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 oligosaccharides 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	266/318 (83%)	0.30	10 (3%) 44 44	14, 24, 40, 54	3 (1%)
1	B	268/318 (84%)	0.80	25 (9%) 16 14	21, 33, 50, 65	1 (0%)
2	P	20/21 (95%)	0.54	0 100 100	32, 40, 65, 73	0
3	V	21/21 (100%)	0.52	0 100 100	28, 40, 53, 63	0
All	All	575/678 (84%)	0.55	35 (6%) 28 28	14, 30, 49, 73	4 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	ALA	5.3
1	B	106	ALA	4.5
1	B	148	ASP	4.5
1	B	112	PRO	4.4
1	B	198	GLY	4.4
1	A	128	TYR	4.3
1	B	128	TYR	4.3
1	A	200	ALA	3.9
1	B	123	SER	3.6
1	A	121	ALA	3.4
1	B	113	GLY	3.2
1	A	123	SER	3.2
1	B	44	LEU	3.1
1	A	127	GLY	2.8
1	B	127	GLY	2.7
1	B	53	THR	2.7
1	B	225	GLY	2.7
1	B	111	LEU	2.6
1	B	109	GLN	2.6
1	A	184	TYR	2.6
1	B	202	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	199	LEU	2.4
1	B	199	LEU	2.4
1	B	200	ALA	2.4
1	B	278	VAL	2.3
1	A	245	GLN	2.3
1	A	106	ALA	2.3
1	B	180	VAL	2.3
1	B	289[A]	HIS	2.2
1	B	140	LEU	2.1
1	B	272	ASN	2.1
1	A	129	SER	2.1
1	B	105	PRO	2.1
1	B	221	ARG	2.0
1	B	122	PRO	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 oligosaccharides 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.