



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 02:28 AM EDT

PDB ID : 8D2M
Title : Covalent Schiff base complex of YedK C2A and abasic DNA
Authors : Eichman, B.F.; Paulin, K.A.
Deposited on : 2022-05-30
Resolution : 1.82 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

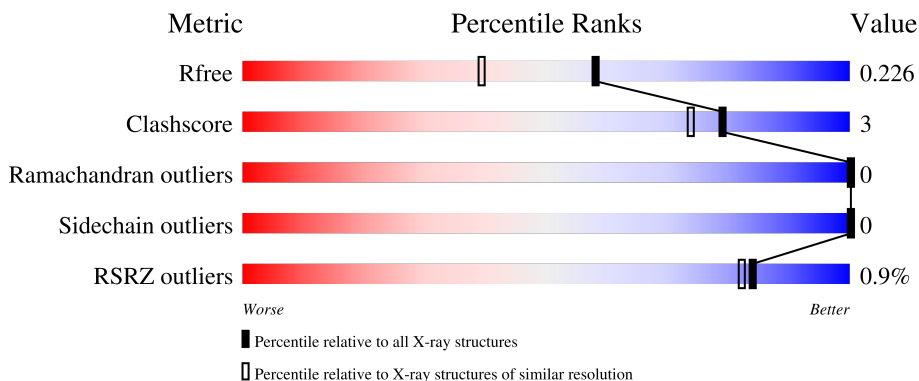
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

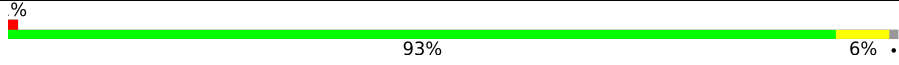
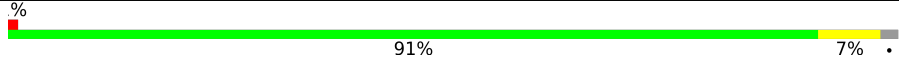
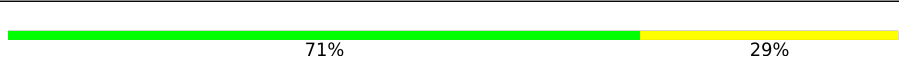
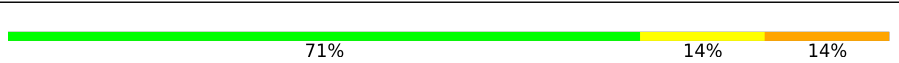
The reported resolution of this entry is 1.82 Å.

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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	227	 93% 6%
1	B	227	 91% 7%
2	C	7	 71% 29%
2	D	7	 71% 14% 14%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7418 atoms, of which 3490 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 Abasic site processing protein YedK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	224	3420	1126	1667	304	318	5	2	2	0
1	B	222	3416	1121	1669	305	316	5	2	3	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	CYS	engineered mutation	UNP P76318
A	223	LEU	-	expression tag	UNP P76318
A	224	GLU	-	expression tag	UNP P76318
A	225	VAL	-	expression tag	UNP P76318
A	226	LEU	-	expression tag	UNP P76318
A	227	PHE	-	expression tag	UNP P76318
A	228	GLN	-	expression tag	UNP P76318
B	2	ALA	CYS	engineered mutation	UNP P76318
B	223	LEU	-	expression tag	UNP P76318
B	224	GLU	-	expression tag	UNP P76318
B	225	VAL	-	expression tag	UNP P76318
B	226	LEU	-	expression tag	UNP P76318
B	227	PHE	-	expression tag	UNP P76318
B	228	GLN	-	expression tag	UNP P76318

- Molecule 2 is a DNA chain called DNA (5'-D>(*GP*TP*CP*(PED)P*GP*GP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	C	7	211	64	77	25	39	6	0	0	0
2	D	7	211	64	77	25	39	6	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total 70	O 70	0	0
3	C	6	Total 6	O 6	0	0
3	B	77	Total 77	O 77	0	0
3	D	7	Total 7	O 7	0	0

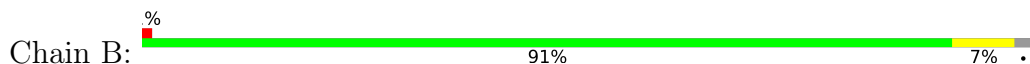
3 Residue-property plots [i](#)

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: Abasic site processing protein YedK



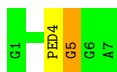
- Molecule 1: Abasic site processing protein YedK



- Molecule 2: DNA (5'-D(*GP*TP*CP*(PED)P*GP*GP*A)-3')



- Molecule 2: DNA (5'-D(*GP*TP*CP*(PED)P*GP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.94Å 41.47Å 82.58Å 90.00° 95.65° 90.00°	Depositor
Resolution (Å)	37.02 – 1.82 37.03 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.02-1.82) 94.1 (37.03-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.82Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.178 , 0.226 0.178 , 0.226	Depositor DCC
R_{free} test set	1852 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7418	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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: PED

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	0.54	0/1815	0.64	0/2472
1	B	0.62	2/1817 (0.1%)	0.69	0/2473
2	C	0.98	0/137	1.01	0/208
2	D	1.28	0/137	1.18	1/208 (0.5%)
All	All	0.64	2/3906 (0.1%)	0.71	1/5361 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12[A]	GLU	CB-CG	5.57	1.62	1.52
1	B	12[B]	GLU	CB-CG	5.57	1.62	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	DG	O4'-C1'-N9	7.31	113.12	108.00

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	A	1753	1667	1669	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1747	1669	1664	9	0
2	C	134	77	78	1	0
2	D	134	77	78	1	0
3	A	70	0	0	0	0
3	B	77	0	0	0	0
3	C	6	0	0	0	0
3	D	7	0	0	0	0
All	All	3928	3490	3489	20	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 3.

All (20) 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:43:LYS:HE2	1:B:141:GLU:OE1	1.97	0.62
1:A:22:ILE:HG23	1:A:54:LEU:CD1	2.36	0.55
1:A:70:LYS:H	1:A:70:LYS:HD2	1.73	0.54
1:B:111:ASP:OD2	1:B:112:LYS:HG2	2.08	0.52
1:A:70:LYS:HB3	1:A:71:PRO:CD	2.42	0.49
1:A:17:LEU:HD22	1:A:125:PRO:HD2	1.98	0.46
2:C:5:DG:H2'	2:C:6:DG:C8	2.50	0.46
1:A:111:ASP:O	1:A:112:LYS:HD3	2.15	0.46
1:A:60:PHE:O	1:A:144:GLY:HA3	2.15	0.45
1:B:43:LYS:CE	1:B:141:GLU:OE1	2.64	0.45
1:B:177:ARG:HB2	1:B:180:ILE:HG12	1.99	0.44
2:D:4:PED:H1'2	2:D:5:DG:H5'	1.99	0.44
1:A:108:LYS:HG3	1:A:110:GLY:O	2.19	0.43
1:A:159:ILE:HD11	1:A:201:TRP:CD1	2.53	0.43
1:B:70:LYS:HB3	1:B:71:PRO:HD2	2.00	0.42
1:B:17:LEU:HD22	1:B:125:PRO:HD2	2.01	0.42
1:B:60:PHE:O	1:B:144:GLY:HA3	2.20	0.41
1:B:70:LYS:HB3	1:B:71:PRO:CD	2.50	0.41
1:A:70:LYS:HD2	1:A:70:LYS:N	2.33	0.41
1:B:88:LYS:HB3	1:B:89:PRO:HD3	2.02	0.41

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	224/227 (99%)	217 (97%)	7 (3%)	0	100	100
1	B	221/227 (97%)	216 (98%)	5 (2%)	0	100	100
All	All	445/454 (98%)	433 (97%)	12 (3%)	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	174/184 (95%)	174 (100%)	0	100	100
1	B	176/184 (96%)	176 (100%)	0	100	100
All	All	350/368 (95%)	350 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	B	55	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 [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	224/227 (98%)	-0.06	2 (0%) 84 82	15, 25, 52, 60	0
1	B	222/227 (97%)	-0.16	2 (0%) 84 82	13, 23, 41, 58	0
2	C	6/7 (85%)	-0.36	0 100 100	27, 28, 39, 40	0
2	D	6/7 (85%)	-0.32	0 100 100	23, 26, 32, 32	0
All	All	458/468 (97%)	-0.11	4 (0%) 84 82	13, 24, 47, 60	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	LEU	3.7
1	B	53	HIS	2.8
1	A	111	ASP	2.7
1	B	111	ASP	2.7

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.