wwPDB X-ray Structure Validation Summary Report (i)

Dec 9, 2023 – 04:22 pm GMT

PDB ID	:	2W4B
Title	:	Epstein-Barr virus alkaline nuclease D203S mutant
Authors	:	Buisson, M.; Geoui, T.; Flot, D.; Tarbouriech, N.; Burmeister, W.P.
Deposited on	:	2008-11-24
Resolution	:	3.50 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 (i) 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 (1)) were used in the production of this report:

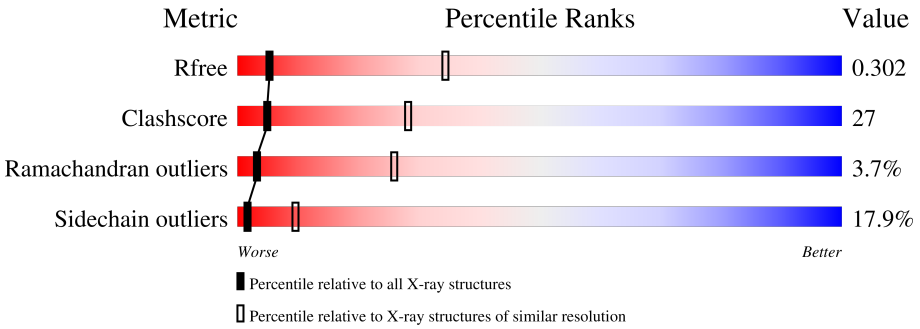
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	470	51% 34% 10%
1	B	470	48% 35% 9% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7041 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 ALKALINE EXONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	1
			3587	2288	605	672	22			
1	B	439	Total	C	N	O	S	0	0	1
			3454	2205	582	645	22			

There are 2 discrepancies between the modelled and reference sequences:

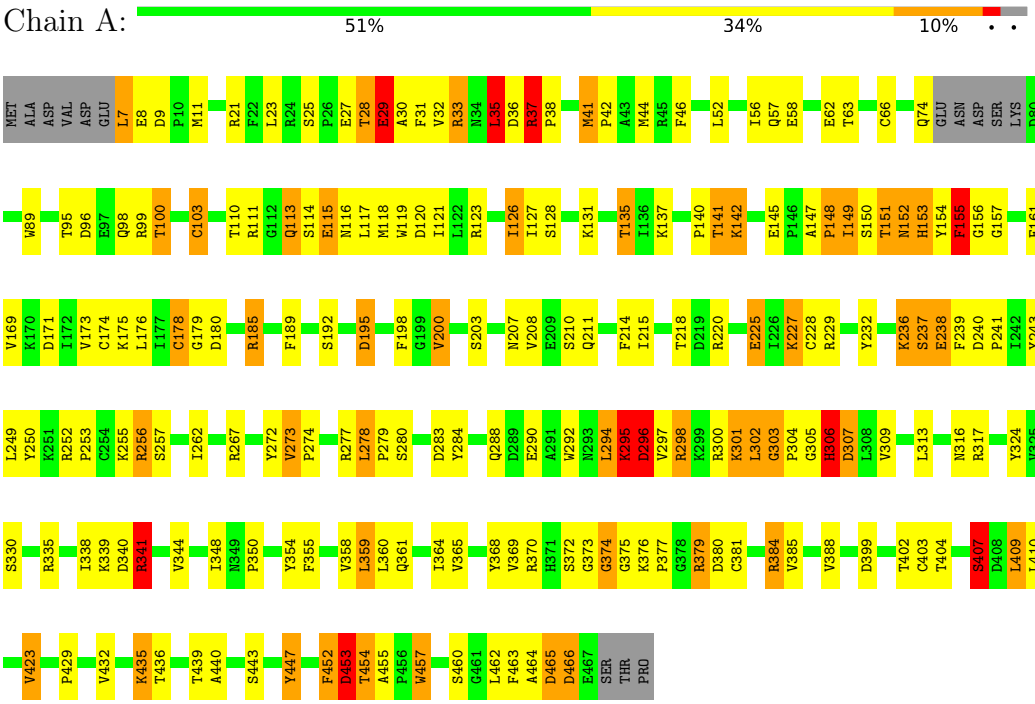
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	ASP	engineered mutation	UNP P03217
B	203	SER	ASP	engineered mutation	UNP P03217

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. 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. 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.

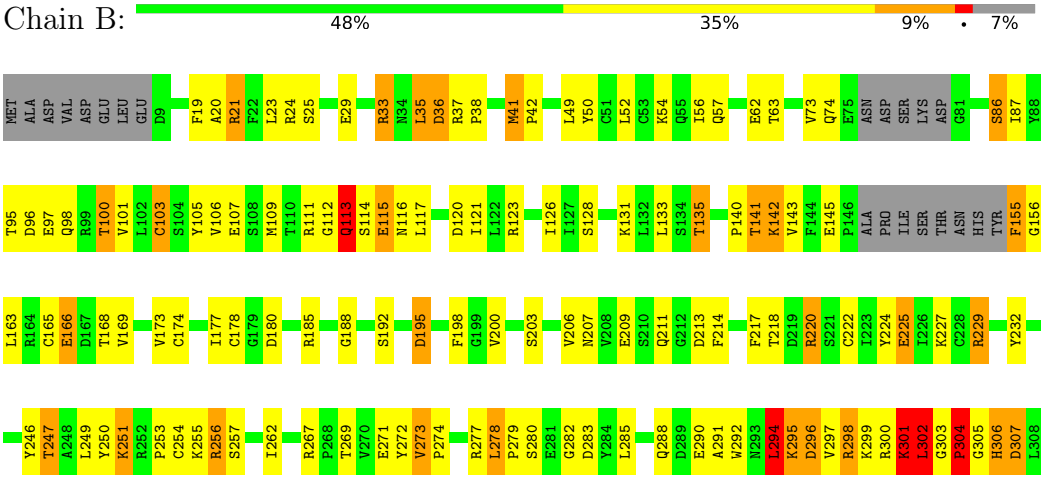
- Molecule 1: ALKALINE EXONUCLEASE

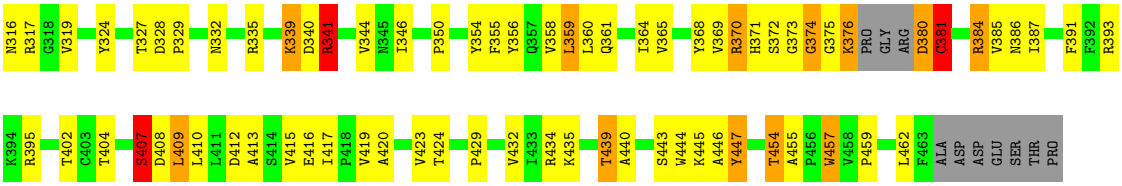
Chain A:



- Molecule 1: ALKALINE EXONUCLEASE

Chain B:




N316 R317 G318 V319 Y324 T327 D328 P329 N332 R335 K339 D340 R341 V344 N345 I346 P350 Y354 F355 Y356 Q357 V358 L359 L360 Q361 I364 V365 Y368 V369 R370 H371 S372 G373 G374 G375 K376 PRO GLY ARG D380 C381 R384 V385 N386 I387 F391 F392 R393
K394 R395 T402 C403 T404 S407 D408 L409 L410 L411 D412 A413 S414 V415 E416 I417 P418 V419 A420 V423 T424 P429 V432 I433 R434 K435 T439 A440 S443 W444 K445 A446 Y447 T454 A455 P456 W457 V458 P459 L462 F463 ALA ASP ASP GLU SER THR PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.51Å 63.79Å 114.13Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	31.19 – 3.50 31.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	84.8 (31.19-3.50) 99.8 (31.19-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.190 , 0.256 0.262 , 0.302	Depositor DCC
R_{free} test set	1295 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	7041	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.18	8/3674 (0.2%)	1.07	14/4987 (0.3%)
1	B	0.99	6/3534 (0.2%)	1.02	19/4791 (0.4%)
All	All	1.09	14/7208 (0.2%)	1.05	33/9778 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	4
All	All	0	12

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	PHE	C-N	-40.57	0.40	1.34
1	A	453	ASP	C-N	-23.24	0.80	1.34
1	B	35	LEU	C-N	-21.17	0.85	1.34
1	B	36	ASP	C-N	-11.74	1.07	1.34
1	B	381	CYS	CB-SG	-9.48	1.66	1.82

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	452	PHE	O-C-N	-19.02	92.27	122.70
1	A	35	LEU	C-N-CA	18.66	168.35	121.70
1	A	452	PHE	C-N-CA	14.54	158.05	121.70
1	A	35	LEU	O-C-N	-13.65	100.86	122.70
1	B	36	ASP	O-C-N	-11.61	104.12	122.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	ILE	Peptide
1	A	150	SER	Peptide
1	A	35	LEU	Peptide
1	A	407	SER	Peptide
1	A	41	MET	Peptide

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	3587	0	3537	204	5
1	B	3454	0	3417	188	1
All	All	7041	0	6954	384	5

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 27.

The worst 5 of 384 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:271:GLU:OE1	1:B:298:ARG:NH1	1.60	1.32
1:A:453:ASP:C	1:A:454:THR:CA	2.00	1.30
1:A:116:ASN:OD1	1:A:117:LEU:N	1.65	1.28
1:B:302:LEU:O	1:B:304:PRO:HD3	1.34	1.26
1:A:95:THR:HG21	1:B:178:CYS:O	1.38	1.23

All (5) 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)
1:A:341:ARG:NH1	1:B:36:ASP:O[2_645]	1.69	0.51
1:A:58:GLU:OE2	1:A:156:GLY:N[2_656]	1.72	0.48
1:A:58:GLU:OE2	1:A:156:GLY:CA[2_656]	1.81	0.39
1:A:58:GLU:OE2	1:A:156:GLY:C[2_656]	1.94	0.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:OE2	1:A:157:GLY:N[2_656]	2.17	0.03

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	452/470 (96%)	370 (82%)	65 (14%)	17 (4%)	3 25
1	B	431/470 (92%)	369 (86%)	46 (11%)	16 (4%)	3 26
All	All	883/940 (94%)	739 (84%)	111 (13%)	33 (4%)	3 26

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	42	PRO
1	A	148	PRO
1	A	295	LYS
1	A	296	ASP

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	400/414 (97%)	325 (81%)	75 (19%)	1 8
1	B	386/414 (93%)	320 (83%)	66 (17%)	2 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	786/828 (95%)	645 (82%)	141 (18%)	2 9

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	302	LEU
1	B	316	ASN
1	B	402	THR
1	A	306	HIS
1	A	302	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	316	ASN
1	B	332	ASN
1	B	371	HIS
1	B	357	GLN
1	B	40	GLN

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:ASP	C	37:ARG	N	1.13
1	B	36:ASP	C	37:ARG	N	1.07
1	B	35:LEU	C	36:ASP	N	0.85
1	A	453:ASP	C	454:THR	N	0.80
1	A	452:PHE	C	453:ASP	N	0.40

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.