



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:42 PM UTC

PDB ID : 3WE1 / pdb_00003we1
Title : Crystal structure of Dengue 4 Envelope protein domain III (ED3)
Authors : Elahi, M.; Islam, M.M.; Noguchi, K.; Yohda, M.; Toh, H.; Kuroda, Y.
Deposited on : 2013-06-27
Resolution : 2.28 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

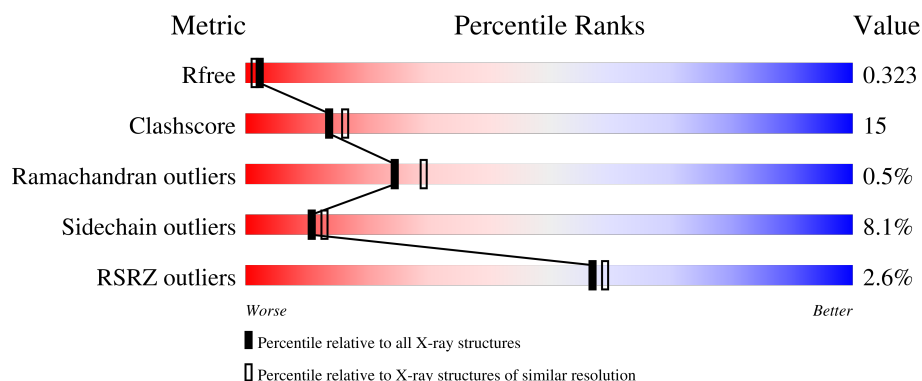
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

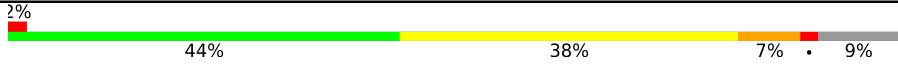
The reported resolution of this entry is 2.28 Å.

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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	107	
1	B	107	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1578 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			736	466	124	142	4			
1	B	97	Total	C	N	O	S	0	0	0
			725	459	120	142	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	GLY	-	expression tag	UNP P09866
A	574	SER	-	expression tag	UNP P09866
B	573	GLY	-	expression tag	UNP P09866
B	574	SER	-	expression tag	UNP P09866

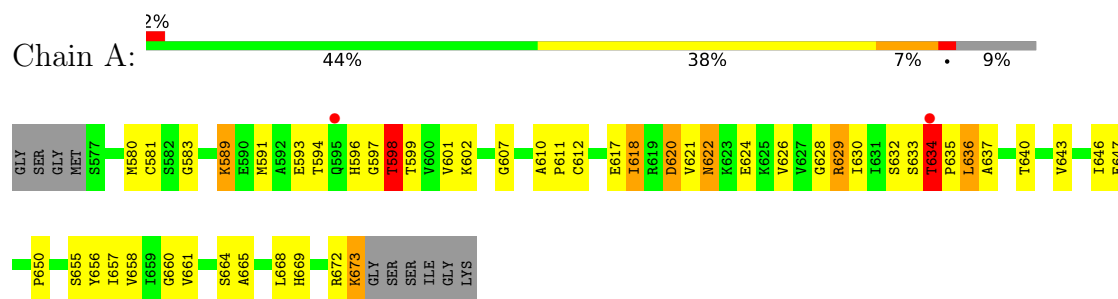
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	76	Total	O	0	0
			76	76		
2	B	41	Total	O	0	0
			41	41		

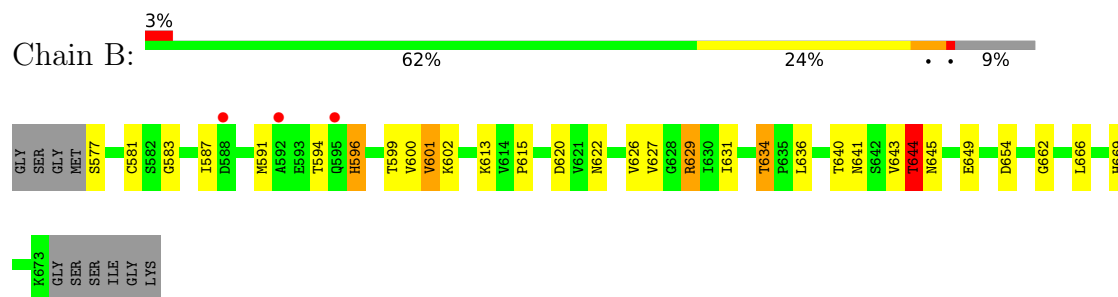
3 Residue-property plots [i](#)

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: Envelope protein E



• Molecule 1: Envelope protein E



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.38Å 91.38Å 73.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.97 – 2.28 9.97 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (9.97-2.28) 98.4 (9.97-2.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.27	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.25 (at 2.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.266 , 0.290 0.295 , 0.323	Depositor DCC
R_{free} test set	733 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	1578	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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

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	2.10	25/750 (3.3%)	1.49	16/1017 (1.6%)
1	B	1.76	3/739 (0.4%)	1.30	7/1006 (0.7%)
All	All	1.94	28/1489 (1.9%)	1.40	23/2023 (1.1%)

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	1
1	B	0	1
All	All	0	2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	PRO	CA-C	9.11	1.63	1.52
1	A	634	THR	C-N	-8.54	1.23	1.33
1	A	672	ARG	C-O	-6.86	1.16	1.24
1	B	626	VAL	C-O	-6.40	1.17	1.24
1	A	661	VAL	C-O	-6.36	1.16	1.23
1	A	607	GLY	C-O	-6.25	1.17	1.23
1	A	650	PRO	C-O	-6.25	1.19	1.25
1	B	644	THR	C-N	6.01	1.41	1.33
1	A	660	GLY	C-O	-6.00	1.15	1.24
1	A	643	VAL	C-O	-5.97	1.17	1.24
1	A	630	ILE	N-CA	5.79	1.53	1.46
1	A	583	GLY	C-O	-5.78	1.16	1.23
1	A	665	ALA	C-O	-5.75	1.16	1.23
1	A	618	ILE	C-O	-5.74	1.18	1.24
1	A	628	GLY	C-O	-5.71	1.16	1.24
1	A	637	ALA	C-O	-5.66	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	630	ILE	C-O	-5.52	1.17	1.23
1	A	636	LEU	C-O	-5.50	1.17	1.23
1	A	640	THR	C-O	-5.21	1.17	1.23
1	B	615	PRO	C-O	-5.17	1.18	1.23
1	A	646	ILE	C-O	-5.16	1.18	1.24
1	A	635	PRO	N-CA	5.16	1.53	1.47
1	A	658	VAL	C-O	-5.14	1.18	1.24
1	A	620	ASP	C-O	-5.12	1.18	1.23
1	A	593	GLU	C-O	-5.12	1.17	1.23
1	A	655	SER	C-O	-5.05	1.17	1.23
1	A	589	LYS	C-O	-5.00	1.18	1.24
1	A	669	HIS	C-O	-5.00	1.17	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	644	THR	CA-C-N	-11.19	107.21	122.99
1	B	644	THR	C-N-CA	-11.19	107.21	122.99
1	A	630	ILE	N-CA-C	9.82	123.05	107.73
1	A	635	PRO	N-CA-C	9.79	125.58	110.80
1	A	622	ASN	N-CA-C	-9.10	98.91	110.19
1	A	628	GLY	CA-C-N	7.63	135.45	122.26
1	A	628	GLY	C-N-CA	7.63	135.45	122.26
1	A	624	GLU	N-CA-C	7.56	122.67	109.96
1	A	634	THR	CA-C-O	7.27	130.12	120.16
1	A	629	ARG	CA-C-N	-7.22	113.34	122.43
1	A	629	ARG	C-N-CA	-7.22	113.34	122.43
1	B	631	ILE	N-CA-C	6.87	116.99	110.53
1	B	581	CYS	O-C-N	6.85	130.76	122.75
1	B	644	THR	O-C-N	6.32	130.81	123.17
1	B	601	VAL	CB-CA-C	-5.97	100.02	110.71
1	A	583	GLY	N-CA-C	5.68	121.86	112.66
1	A	581	CYS	CA-C-N	5.68	130.34	120.68
1	A	581	CYS	C-N-CA	5.68	130.34	120.68
1	A	598	THR	N-CA-C	5.64	118.17	110.55
1	A	633	SER	CA-C-O	5.31	126.97	120.92
1	A	628	GLY	CA-C-O	5.29	125.58	119.13
1	B	583	GLY	N-CA-C	5.08	120.37	112.60
1	A	632	SER	O-C-N	5.08	129.11	122.87

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	597	GLY	Peptide
1	B	644	THR	Mainchain

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	736	0	733	23	0
1	B	725	0	699	19	0
2	A	76	0	0	1	0
2	B	41	0	0	1	0
All	All	1578	0	1432	41	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 15.

All (41) 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:A:598:THR:HG21	1:A:647:GLU:OE2	1.60	1.01
1:A:591:MET:HE3	1:A:668:LEU:HD13	1.66	0.77
1:B:629:ARG:HD3	1:B:649:GLU:O	1.87	0.75
1:A:591:MET:HE1	1:A:657:ILE:HD13	1.68	0.73
1:B:654:ASP:OD2	1:B:669:HIS:NE2	2.20	0.71
1:A:629:ARG:HB2	2:A:720:HOH:O	1.90	0.70
1:B:602:LYS:HA	1:B:644:THR:O	1.95	0.66
1:B:640:THR:O	1:B:641:ASN:HB2	1.97	0.64
1:B:644:THR:CG2	1:B:645:ASN:N	2.62	0.62
1:A:612:CYS:O	1:A:636:LEU:HD12	2.04	0.58
1:A:626:VAL:HG12	1:A:629:ARG:HG2	1.85	0.58
1:B:594:THR:HG1	1:B:596:HIS:HD1	1.50	0.57
1:B:634:THR:HG22	2:B:720:HOH:O	2.04	0.57
1:A:598:THR:HG23	1:A:647:GLU:HG3	1.87	0.56
1:B:602:LYS:CD	1:B:645:ASN:OD1	2.54	0.55
1:B:644:THR:HG22	1:B:645:ASN:N	2.21	0.55
1:B:643:VAL:HG12	1:B:644:THR:N	2.22	0.55
1:A:591:MET:HG3	1:A:601:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:THR:OG1	1:B:596:HIS:ND1	2.38	0.55
1:A:594:THR:CG2	1:A:598:THR:HG22	2.40	0.52
1:A:591:MET:HE3	1:A:668:LEU:CD1	2.40	0.51
1:A:598:THR:CG2	1:A:647:GLU:HG3	2.43	0.49
1:A:589:LYS:HB3	1:A:602:LYS:HB2	1.94	0.49
1:B:587:ILE:HD11	1:B:666:LEU:HD13	1.94	0.49
1:B:591:MET:HG2	1:B:599:THR:HB	1.95	0.47
1:A:620:ASP:O	1:A:622:ASN:O	2.32	0.47
1:A:610:ALA:HA	1:A:611:PRO:C	2.40	0.46
1:A:598:THR:HG21	1:A:647:GLU:CD	2.34	0.46
1:A:618:ILE:N	1:A:618:ILE:HD12	2.30	0.46
1:B:620:ASP:OD1	1:B:622:ASN:N	2.48	0.45
1:B:591:MET:HA	1:B:600:VAL:O	2.15	0.45
1:A:594:THR:HG21	1:A:598:THR:HG22	1.99	0.44
1:B:613:LYS:HB2	1:B:613:LYS:HE3	1.75	0.43
1:A:617:GLU:C	1:A:618:ILE:HD12	2.44	0.43
1:A:580:MET:O	1:B:662:GLY:N	2.51	0.42
1:A:656:TYR:HA	1:A:668:LEU:O	2.20	0.42
1:A:599:THR:O	1:A:647:GLU:HA	2.20	0.41
1:A:673:LYS:HA	1:A:673:LYS:HD3	1.83	0.41
1:B:640:THR:O	1:B:641:ASN:CB	2.67	0.41
1:A:612:CYS:C	1:A:636:LEU:HD12	2.46	0.41
1:B:643:VAL:CG1	1:B:644:THR:N	2.83	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	95/107 (89%)	93 (98%)	1 (1%)	1 (1%)	11	11
1	B	95/107 (89%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	190/214 (89%)	185 (97%)	4 (2%)	1 (0%)	24	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	634	THR

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	A	82/90 (91%)	76 (93%)	6 (7%)	13	16
1	B	78/90 (87%)	71 (91%)	7 (9%)	9	10
All	All	160/180 (89%)	147 (92%)	13 (8%)	11	13

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	596	HIS
1	A	598	THR
1	A	621	VAL
1	A	634	THR
1	A	664	SER
1	A	673	LYS
1	B	577	SER
1	B	596	HIS
1	B	601	VAL
1	B	627	VAL
1	B	629	ARG
1	B	634	THR
1	B	636	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	663	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 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	97/107 (90%)	0.08	2 (2%) 63 65	23, 33, 44, 49	0
1	B	97/107 (90%)	0.28	3 (3%) 51 53	25, 40, 52, 63	0
All	All	194/214 (90%)	0.18	5 (2%) 57 59	23, 37, 49, 63	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	634	THR	3.3
1	A	595	GLN	3.2
1	B	588	ASP	2.2
1	B	595	GLN	2.1
1	B	592	ALA	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 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.