



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:10 PM UTC

PDB ID : 5EDP / pdb_00005edp
Title : EGFR kinase (T790M/L858R) apo
Authors : Eigenbrot, C.; Yu, C.
Deposited on : 2015-10-21
Resolution : 2.90 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

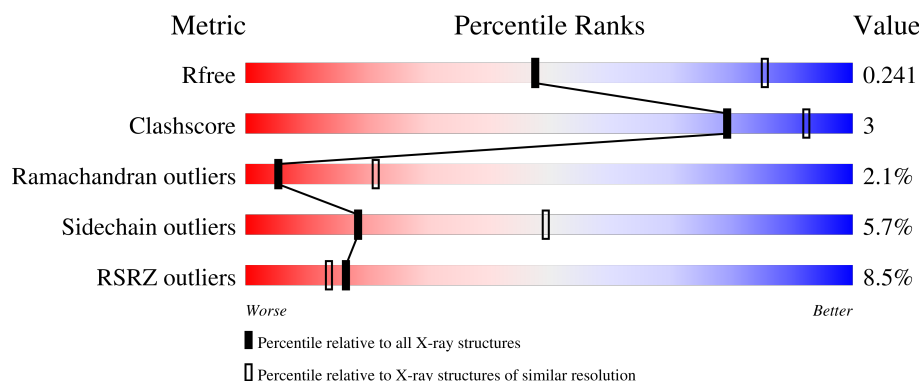
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

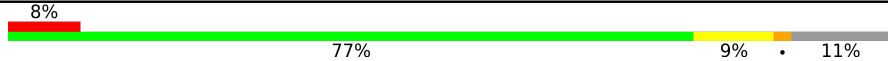
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	331	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2366 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2366	1522	399	428	17			

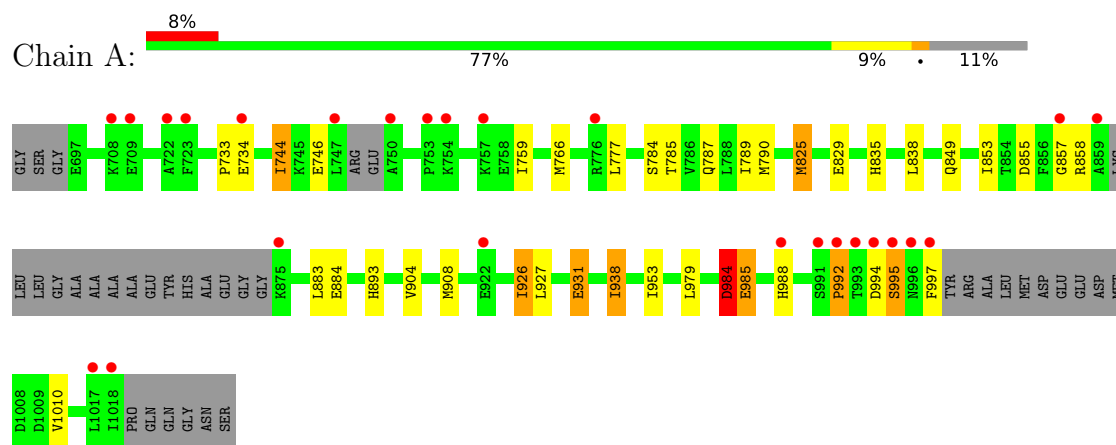
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	694	GLY	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	858	ARG	LEU	engineered mutation	UNP P00533
A	865	ALA	GLU	engineered mutation	UNP P00533
A	866	ALA	GLU	engineered mutation	UNP P00533
A	867	ALA	LYS	engineered mutation	UNP P00533
A	1023	ASN	-	expression tag	UNP P00533
A	1024	SER	-	expression tag	UNP P00533

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: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	148.85Å 148.85Å 148.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.07 – 2.90 47.07 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.07-2.90) 100.0 (47.07-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.244 0.204 , 0.241	Depositor DCC
R_{free} test set	530 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2366	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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	0.81	1/2417 (0.0%)	1.29	8/3271 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	825	MET	SD-CE	-8.32	1.58	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	858	ARG	N-CA-C	-6.45	105.04	114.39
1	A	857	GLY	CA-C-N	6.15	131.38	121.98
1	A	857	GLY	C-N-CA	6.15	131.38	121.98
1	A	984	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	992	PRO	CA-C-N	5.82	131.01	121.58
1	A	992	PRO	C-N-CA	5.82	131.01	121.58
1	A	733	PRO	CA-C-N	5.36	131.78	121.54
1	A	733	PRO	C-N-CA	5.36	131.78	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2366	0	2405	13	0
All	All	2366	0	2405	13	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 (13) 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:825:MET:HE1	1:A:835:HIS:HD2	1.69	0.57
1:A:984:ASP:O	1:A:985:GLU:HG2	2.09	0.53
1:A:829:GLU:HA	1:A:893:HIS:CE1	2.43	0.52
1:A:825:MET:HE3	1:A:838:LEU:HD13	1.91	0.51
1:A:995:SER:C	1:A:997:PHE:H	2.18	0.51
1:A:825:MET:HE1	1:A:835:HIS:CD2	2.47	0.49
1:A:904:VAL:O	1:A:908:MET:HG2	2.16	0.45
1:A:938:ILE:HD12	1:A:979:LEU:HD22	1.97	0.45
1:A:744:ILE:HG23	1:A:789:ILE:HG13	1.99	0.45
1:A:926:ILE:HG23	1:A:931:GLU:HB3	1.99	0.45
1:A:883:LEU:HD22	1:A:953:ILE:HD12	2.01	0.43
1:A:766:MET:HB3	1:A:777:LEU:HB2	2.02	0.41
1:A:746:GLU:HB3	1:A:787:GLN:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	287/331 (87%)	268 (93%)	13 (4%)	6 (2%)	5	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	734	GLU
1	A	985	GLU
1	A	988	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	995	SER
1	A	994	ASP
1	A	992	PRO

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	263/287 (92%)	248 (94%)	15 (6%)	18	49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	744	ILE
1	A	759	ILE
1	A	784	SER
1	A	785	THR
1	A	790	MET
1	A	849	GLN
1	A	853	ILE
1	A	855	ASP
1	A	884	GLU
1	A	926	ILE
1	A	927	LEU
1	A	931	GLU
1	A	938	ILE
1	A	984	ASP
1	A	1010	VAL

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	700	ASN
1	A	849	GLN
1	A	888	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	893	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	295/331 (89%)	0.34	25 (8%) 16 14	46, 69, 118, 139	6 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1018	ILE	7.0
1	A	747	LEU	5.5
1	A	996	ASN	5.5
1	A	734	GLU	4.8
1	A	1017	LEU	4.7
1	A	859	ALA	4.4
1	A	988	HIS	4.1
1	A	723	PHE	3.4
1	A	997	PHE	3.3
1	A	993	THR	3.3
1	A	857	GLY	3.0
1	A	991	SER	2.8
1	A	750	ALA	2.7
1	A	722	ALA	2.7
1	A	922	GLU	2.6
1	A	753	PRO	2.6
1	A	994	ASP	2.4
1	A	992	PRO	2.3
1	A	709	GLU	2.2
1	A	754	LYS	2.2
1	A	995	SER	2.2
1	A	757	LYS	2.2
1	A	776	ARG	2.2
1	A	875	LYS	2.0
1	A	708	LYS	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.