



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2EB2 / pdb_00002eb2
Title : Crystal structure of mutated EGFR kinase domain (G719S)
Authors : Yoshikawa, S.; Kukimoto-Niino, M.; Chen, L.; Liu, Z.J.; Wang, B.C.; Shirouzu, M.; Senba, K.; Yamamoto, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-02-06
Resolution : 2.50 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
Xtrriage (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

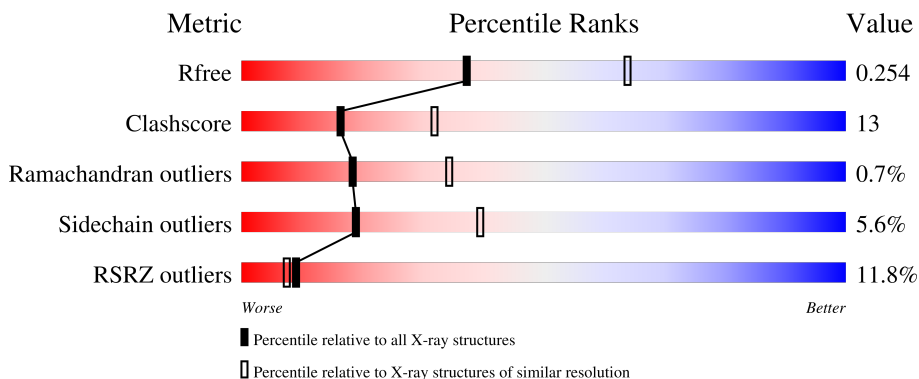
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	334	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2459 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
			Total	C	N	O	S			
1	A	305	2443	1569	412	445	17	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	689	GLY	-	expression tag	UNP P00533
A	690	ALA	-	expression tag	UNP P00533
A	691	MET	-	expression tag	UNP P00533
A	692	GLY	-	expression tag	UNP P00533
A	693	ILE	-	expression tag	UNP P00533
A	694	ARG	-	expression tag	UNP P00533
A	719	SER	GLY	SEE REMARK 999	UNP P00533

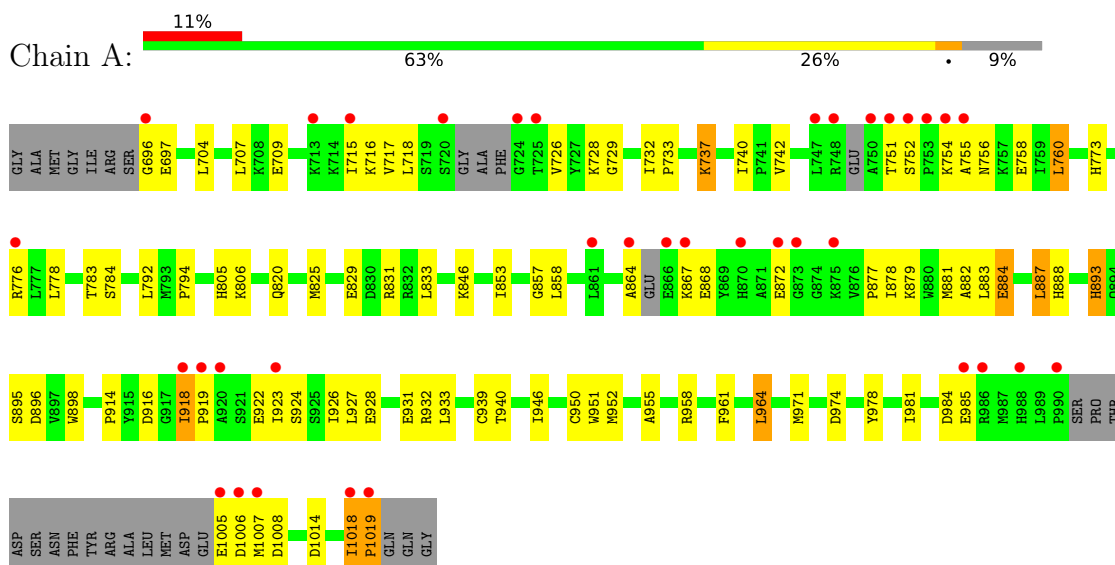
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		

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	145.47Å 145.47Å 145.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 – 2.50 46.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.00-2.50) 100.0 (46.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.21 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.253 0.200 , 0.254	Depositor DCC
R_{free} test set	1755 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2459	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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](#)

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	0.61	0/2493	1.02	10/3370 (0.3%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	740	ILE	N-CA-C	6.28	114.32	107.60
1	A	946	ILE	CB-CA-C	-5.92	104.27	112.02
1	A	974	ASP	CA-C-N	5.66	125.12	119.24
1	A	974	ASP	C-N-CA	5.66	125.12	119.24
1	A	939	CYS	N-CA-C	5.38	118.39	109.46
1	A	895	SER	N-CA-C	-5.15	105.85	111.82
1	A	893	HIS	N-CA-C	-5.07	105.84	111.36
1	A	726	VAL	N-CA-C	5.06	115.87	108.58
1	A	697	GLU	N-CA-C	-5.04	107.12	114.12
1	A	940	THR	N-CA-C	-5.02	104.23	110.41

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	2443	0	2485	64	0
2	A	16	0	0	0	0
All	All	2459	0	2485	64	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 13.

All (64) 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:1018:ILE:HB	1:A:1019:PRO:HD2	1.15	1.09
1:A:1018:ILE:HB	1:A:1019:PRO:CD	1.87	1.04
1:A:918:ILE:H	1:A:918:ILE:HD12	1.22	0.99
1:A:737:LYS:HE2	1:A:737:LYS:HA	1.44	0.99
1:A:1005:GLU:HB3	1:A:1007:MET:HE3	1.59	0.82
1:A:887:LEU:HB3	1:A:888:HIS:CD2	2.19	0.77
1:A:882:ALA:HB1	1:A:884:GLU:OE2	1.87	0.73
1:A:1018:ILE:CB	1:A:1019:PRO:HD2	2.08	0.68
1:A:971:MET:HG2	1:A:978:TYR:CG	2.33	0.64
1:A:776:ARG:HH11	1:A:776:ARG:HG3	1.63	0.63
1:A:971:MET:HG2	1:A:978:TYR:CD1	2.36	0.60
1:A:754:LYS:O	1:A:758:GLU:HG3	2.01	0.60
1:A:751:THR:HB	1:A:756:ASN:HD21	1.66	0.60
1:A:857:GLY:C	1:A:858:LEU:HD12	2.28	0.59
1:A:737:LYS:HA	1:A:737:LYS:CE	2.26	0.57
1:A:783:THR:O	1:A:784:SER:C	2.47	0.56
1:A:1006:ASP:O	1:A:1007:MET:HE2	2.04	0.56
1:A:924:SER:O	1:A:928:GLU:HG3	2.04	0.56
1:A:985:GLU:H	1:A:985:GLU:CD	2.13	0.55
1:A:952:MET:HB2	1:A:958:ARG:HG2	1.89	0.55
1:A:829:GLU:HG3	1:A:893:HIS:CD2	2.41	0.55
1:A:888:HIS:CD2	1:A:888:HIS:N	2.77	0.52
1:A:918:ILE:HG21	1:A:926:ILE:HD12	1.91	0.52
1:A:696:GLY:HA3	1:A:864:ALA:H	1.75	0.51
1:A:715:ILE:HG12	1:A:729:GLY:HA2	1.92	0.51
1:A:918:ILE:H	1:A:918:ILE:CD1	2.01	0.49
1:A:918:ILE:HD12	1:A:918:ILE:N	2.06	0.49
1:A:878:ILE:HA	1:A:881:MET:SD	2.53	0.49
1:A:1018:ILE:O	1:A:1019:PRO:C	2.55	0.49
1:A:756:ASN:O	1:A:760:LEU:HD22	2.13	0.48
1:A:858:LEU:HD12	1:A:858:LEU:N	2.28	0.48
1:A:893:HIS:O	1:A:896:ASP:HB2	2.13	0.48
1:A:717:VAL:HG12	1:A:718:LEU:N	2.29	0.47
1:A:805:HIS:O	1:A:806:LYS:C	2.57	0.47
1:A:716:LYS:CG	1:A:728:LYS:HD3	2.44	0.47
1:A:825:MET:SD	1:A:853:ILE:HD13	2.54	0.47
1:A:918:ILE:HG12	1:A:926:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:LEU:C	1:A:833:LEU:HD23	2.41	0.46
1:A:952:MET:HE2	1:A:952:MET:HA	1.98	0.46
1:A:879:LYS:HD3	1:A:914:PRO:O	2.16	0.46
1:A:961:PHE:HA	1:A:964:LEU:HD23	1.98	0.46
1:A:776:ARG:HH11	1:A:776:ARG:CG	2.25	0.45
1:A:919:PRO:HD2	1:A:922:GLU:OE2	2.18	0.44
1:A:776:ARG:CG	1:A:776:ARG:NH1	2.82	0.43
1:A:752:SER:C	1:A:754:LYS:N	2.75	0.43
1:A:922:GLU:O	1:A:923:ILE:C	2.61	0.43
1:A:950:CYS:O	1:A:958:ARG:HD2	2.18	0.42
1:A:752:SER:O	1:A:755:ALA:N	2.52	0.42
1:A:955:ALA:HA	1:A:958:ARG:CZ	2.49	0.42
1:A:716:LYS:HG2	1:A:728:LYS:HD3	2.01	0.42
1:A:732:ILE:O	1:A:733:PRO:C	2.62	0.42
1:A:981:ILE:O	1:A:984:ASP:HB2	2.19	0.42
1:A:877:PRO:O	1:A:881:MET:HG3	2.19	0.42
1:A:846:LYS:NZ	1:A:1014:ASP:OD2	2.46	0.42
1:A:792:LEU:O	1:A:794:PRO:HD3	2.20	0.42
1:A:867:LYS:HG3	1:A:868:GLU:HG2	2.01	0.42
1:A:933:LEU:HB2	1:A:951:TRP:CH2	2.55	0.41
1:A:717:VAL:CG1	1:A:718:LEU:N	2.84	0.41
1:A:931:GLU:O	1:A:932:ARG:HD3	2.20	0.41
1:A:773:HIS:CE1	1:A:820:GLN:HG2	2.56	0.41
1:A:1018:ILE:CB	1:A:1019:PRO:CD	2.72	0.41
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.56	0.41
1:A:709:GLU:CG	1:A:783:THR:HG21	2.50	0.40
1:A:831:ARG:HA	1:A:831:ARG:HD3	1.83	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	295/334 (88%)	275 (93%)	18 (6%)	2 (1%)	18 34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	ILE
1	A	916	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	270/292 (92%)	255 (94%)	15 (6%)	19 39

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

Mol	Chain	Res	Type
1	A	704	LEU
1	A	707	LEU
1	A	737	LYS
1	A	742	VAL
1	A	760	LEU
1	A	778	LEU
1	A	872	GLU
1	A	883	LEU
1	A	884	GLU
1	A	887	LEU
1	A	918	ILE
1	A	927	LEU
1	A	964	LEU
1	A	1008	ASP
1	A	1019	PRO

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	756	ASN
1	A	773	HIS
1	A	888	HIS
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

6.1 Protein, DNA and RNA chains

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	305/334 (91%)	0.44	36 (11%) 9 7	27, 49, 115, 139	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1018	ILE	7.9
1	A	724	GLY	6.5
1	A	1019	PRO	6.4
1	A	867	LYS	5.4
1	A	748	ARG	5.4
1	A	864	ALA	5.1
1	A	750	ALA	4.8
1	A	751	THR	4.7
1	A	747	LEU	4.5
1	A	720	SER	4.1
1	A	1005	GLU	3.9
1	A	990	PRO	3.9
1	A	696	GLY	3.8
1	A	988	HIS	3.5
1	A	753	PRO	3.3
1	A	918	ILE	3.2
1	A	752	SER	3.1
1	A	1006	ASP	3.0
1	A	715	ILE	2.9
1	A	725	THR	2.8
1	A	873	GLY	2.8
1	A	872	GLU	2.6
1	A	754	LYS	2.6
1	A	776	ARG	2.5
1	A	919	PRO	2.5
1	A	861	LEU	2.5
1	A	1007	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	986	ARG	2.4
1	A	985	GLU	2.4
1	A	875	LYS	2.3
1	A	870	HIS	2.2
1	A	866	GLU	2.2
1	A	920	ALA	2.1
1	A	923	ILE	2.1
1	A	713	LYS	2.1
1	A	755	ALA	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.